

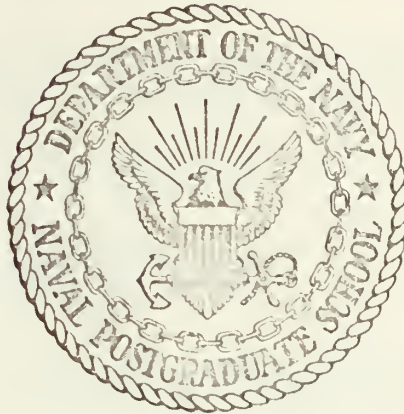
APPLICATION OF THE HARRIS EXPANSION METHOD  
TO THE ELASTIC S-WAVE SCATTERING OF ELECTRONS  
BY HYDROGEN ATOMS AND BY SINGLY IONIZED HELIUM

Hugh Brasher Haskell

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# NAVAL POSTGRADUATE SCHOOL

## Monterey, California



# THESIS

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Hugh Brasher Haskell

Thesis Advisor:

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December 1972

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by Hydrogen Atoms and by Singly Ionized Helium

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DOCTOR OF PHILOSOPHY

from the  
NAVAL POSTGRADUATE SCHOOL  
December 1972



## ABSTRACT

The Harris expansion method is applied to the elastic s-wave scattering of low energy electrons from hydrogen atoms and singly ionized helium atoms. The trial wave functions are Hylleraas functions of 22, 34, 50 and 70 parameters. It is found that reasonably accurate values of e-H phase shifts can be calculated but that e-He<sup>+</sup> phase shifts are substantially less reliable. It is shown that the Harris method gives an accurate depiction of the location, but not the width, of the scattering resonances. Singlet and triplet s-wave phase shifts for e-H and e-He<sup>+</sup> scattering are compared with the results of other calculations and H<sup>-</sup> and He S state energy levels including the auto-ionizing levels are presented and compared with other calculations and with experiment. It is tentatively concluded that the Harris method does not work on systems whose long range potential is of the Coulomb type.



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## ACKNOWLEDGEMENT

It is a pleasure to acknowledge the continued support and encouragment of Professor Otto Heinz and also that of Professor Robert Armstead under whose direction this work has proceeded. Dr. D.E. Harrison, Jr., provided several helpful suggestions regarding techniques of numerical integration. Professor A.H. Stroud of Texas A & M University kindly provided the computer program by which the sample points and weight factors for the Gauss-Legendre numerical integrations were generated. The numerical calculations were performed on the IBM 360/67 computer of the Naval Postgraduate School Computer Facility, whose personnel were most helpful on several occasions. Last but not least, the author wishes to gratefully acknowledge the continued moral support of his wife, who perservered through some very trying times.



## I. INTRODUCTION

The quantum theory of scattering has had a long and fruitful history, beginning with the very origins of quantum theory. Its extensive application to atomic collisions is indicated by the large number of texts, monographs and reviews of that subject presently in print [1]. More recently the wide availability of high speed electronic computers has given additional impetus to the subject. New methods have been devised and older ones refurbished to take advantage of the computational power now at the disposal of virtually every investigator in the field. Parallel to the development of computer technology has been the application of powerful variational techniques to the scattering problem.

Variational methods have held a distinguished place in mathematical physics since the days of the Bernoullis. Perhaps no technique has had wider application and thus it is no surprise that it has proven a powerful tool in scattering theory as well. Its first application to atomic scattering by Hulthen in 1944 [2], followed shortly by Kohn [3] and Lippman and Schwinger [4] has led to extensive applications to all areas of scattering theory [5]. One difficulty that arose with the Kohn and related methods however, was the appearance of spurious singularities in the calculated phase shifts. While not fatal to the method they were annoying and some considerable effort has been expended in attempts to explain these singularities by Schwartz [6] and others [7,8,9]. By working to exploit rather than eliminate the singularities,



Harris [10] developed an expansion technique that has yielded very reliable results to date. While this scheme involves some computational simplifications over the Kohn method it too is not without disadvantages, which are dealt with in some detail below.

Formal solutions abound to the scattering problem, ranging from the Born approximation and partial wave analysis to the Green's function methods developed by Schwinger [11], but accurate solutions to "real" problems beyond the realm of potential scattering are relatively few, owing principally to the complexity of the problem when one permits the scattering center to have structure. Even the simplest of "non-trivial" scattering problems, that of electrons or positrons incident elastically on ground state hydrogen atoms is already a "many body" problem and thus not subject to solution in closed form.

It is the purpose of this thesis to investigate the application of the method developed by Harris to the problem of the elastic scattering of low energy electrons from hydrogen atoms and from singly ionized helium. Both have been attempted several times previously by various other methods, most notably in the case of hydrogen by Schwartz, whose definitive calculation was published in 1961 [12] and more recently by Callaway and his collaborators in 1969 and 1970 [13,14], and by Adelman and Reinhardt [15] and Truhlar and Smith [16] in 1972. Because of the more complex nature of the interaction in the case of singly ionized helium and a paucity of experimental data for comparison these calculations have not been as extensively pursued. The earliest attempt was by Bransden and Dalgarno in 1953 [17] and the most recent by Burke and Taylor in 1966 [18].





With the exception of Schwartz' work most of the important calculations of these problems have used the algebraic close coupling approximation [19] wherein the trial wave function is made up at least in part of a combination of the first few bound state orbitals of the target atom. Such a scheme has earned a deserved reputation for accuracy and rapid convergence, however from a philosophical point of view it suffers because its application requires some a priori knowledge of the detailed structure of the target particle. On the other hand Schwartz, in his calculation, made use of an ever increasing set of those functions first used by Hylleraas in his famous calculation of the ground state energy of helium [20]. This method makes no approximations other than those required by the use of a finite rather than an infinite basis space in which to work<sup>1</sup>.

It was in the spirit of Schwartz' work that the present project was undertaken. It was hoped that by utilizing the Hylleraas type functions in a calculation of electron-helium ion scattering that a more accurate and complete compilation of s-wave phase shifts would be obtained. As will be seen below such hopes were not realized, however it is hoped that the reporting of such results

---

<sup>1</sup>This is not strictly true. Electron capture by the scattering center is usually neglected in calculations of this type, and is neglected also in the calculation reported in this thesis. To incorporate capture requires including terms in the potential involving the interaction of the electrons with the electromagnetic field in order to account for the creation of the necessary photons and is properly a problem in quantum electrodynamics. The reported cross sections for capture in the system under consideration here are small compared to the elastic scattering cross sections and usually may be safely neglected.



as were obtained will provide incentive for others to seek an explanation of the apparently anomalous results for helium ion scattering herein reported.

In Section II a brief development of the partial wave method of scattering theory will be presented including the modifications required in the presence of the long range Coulomb force followed by a description of the Kohn method. Last will be a more detailed description of the Harris method and its application to elastic electron scattering by single-electron atoms and ions. In Section III the results of the numerical calculations are presented for both atomic hydrogen and singly ionized helium along with a discussion of these results and comparison with those of other workers. An important by-product of the Harris method is the calculation of the bound state energy levels of the corresponding two-electron system. Results of these calculations for  $H^-$  and He are also presented in Section III. Most of the detailed calculations as well as discussion of the numerical methods employed are deferred to the appendices.



## II. EXPANSION TECHNIQUES IN SCATTERING THEORY

In this section will be presented a brief outline of the method of partial wave analysis [21] for the case of elastic atomic scattering. Part B will briefly present the Kohn method and in part C the Harris method will be developed in some detail along with its application to elastic  $\text{He}^+$  scattering of electrons. The system of units used throughout will be those in which  $m$  (electron mass),  $\hbar$  (Planck's constant) and  $e$  (electronic charge) all equal unity. In such a system the unit of energy is equal to twice the ground state energy of hydrogen (i.e., 27.2 eV), and momenta are written in terms of the wave number,  $k$ , such that  $E = k^2/2$ . It will be assumed that the nuclear mass, be it hydrogen or helium, is infinitely large compared to that of the electrons.

### A. PARTIAL WAVES AND PHASE SHIFTS

Let a beam of particles of momentum  $\vec{k}$  fall upon a spherically symmetric potential  $V(r)$ . Taking the scattering center as the coordinate origin and the direction of  $\vec{k}$  as the angular axis the wave function of the outgoing beam far from the coordinate center will be proportional to the sum of the wave function of the incident beam, represented by the plane wave  $\exp(i\vec{k}\cdot\vec{r})$  and a modified spherical wave,  $f(\theta)\exp(ikr)/r$ , representing the scattered portion of the incident beam. For proof that solutions to the Schroedinger equation of the form

$$\Psi(r) \xrightarrow{r \rightarrow \infty} e^{i\vec{k}\cdot\vec{r}} + f(\theta)e^{ikr}/r \quad (1)$$



exist, the reader is directed to reference 21 (p. 220 ff). The differential scattering cross-section is defined to be

$$\sigma(\theta)d\Omega = \frac{\text{Number of particles per unit time scattered into the solid angle element } d\Omega \text{ at } \theta}{\text{Total Incident Flux}} \quad (2)$$

where the particle flux is defined to be

$$\vec{\varphi} \propto \frac{1}{2i} (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*). \quad (3)$$

Putting (3) into (2) gives

$$\sigma(\theta)d\Omega = \frac{\vec{\varphi}_s \cdot \vec{ds}}{\varphi_o} = \frac{\vec{\varphi}_s \cdot \hat{r} r^2}{\varphi_o} d\Omega \quad (4)$$

where  $\vec{ds}$  is the element of surface area at the detector and  $\hat{r}$  is a unit vector in the direction of the scattered flux.  $\varphi_o$  and  $\varphi_s$  represent respectively the flux arising from the first and second terms of (1), respectively. Because of the scalar product in (4) only the radial part of the scattered wave function contributes to the scattered flux. Evaluating  $\varphi_s$  and  $\varphi_o$  from (3) and applying them to (4) leads immediately to

$$\sigma(\theta)d\Omega = |f(\theta)|^2 d\Omega. \quad (5)$$

It remains then to exhibit a means of calculating  $f(\theta)$  to complete the connection between theory and experiment. Such a means is the method of partial wave analysis. The most general solution to the Schroedinger equation in the case of axial symmetry is

$$\Psi(r) = \sum_{\ell=0}^{\infty} a_{\ell} \frac{u_{\ell}(r)}{r} Y_{\ell}^0(\theta) \quad (6)$$





where  $Y_{\ell}^0(\theta)$  is the spherical harmonic of order zero. The index  $\ell$  represents the angular momentum quantum number. Each radial function satisfies an equation of the form

$$\left[ -\frac{1}{2r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + V(r) + \frac{\ell(\ell+1)}{2r^2} - \frac{k^2}{2} \right] \frac{u_{\ell}(r)}{r} = 0. \quad (7)$$

If  $V(r)$  goes to zero fast enough at large  $r$  there will be a region outside of which its effects can be neglected. Since  $u_{\ell}(r)$  is a function of  $r$  only, equation (7) can be rewritten

$$u'' + [k^2 - 2V(r) - \ell(\ell+1)/r^2] u = 0$$

and since the last two terms tend to zero for large  $r$  it is reasonable to assume that any solution  $u$  tends to the form  $A \sin(kr + \epsilon)$  for large  $r$ . If this be so,  $u$  must have the form  $f(r)e^{ikr}$  where  $f(r)$  is approximately constant for large  $r$ , and (7) reduces to

$$f'' + 2ikf' - [2V(r) + \ell(\ell+1)/r^2] f = 0$$

and for large  $r$ , if  $f$  is nearly constant  $f'' \ll kf'$  and this equation can be approximately integrated, giving

$$2ik \ln f = \int [2V(r) + \ell(\ell+1)/r^2] dr$$

and the right hand side tends to a constant for large  $r$  only if  $V(r)$  goes to zero faster than  $1/r$  (ref. 22, p. 23).

In the region where  $V(r)$  can be neglected equation (7) reduces to the spherical Bessel equation whose solutions are

$$\frac{u_{\ell}(r)}{r} = A_{\ell} j_{\ell}(kr) + B_{\ell} n_{\ell}(kr) \quad (8)$$



where  $j_\ell(kr)$  and  $n_\ell(kr)$  are the spherical Bessel and Neumann functions, respectively [23] whose asymptotic forms are

$$j_\ell(kr) \xrightarrow{r \rightarrow \infty} \sin(kr - \ell \pi/2)/kr$$

$$n_\ell(kr) \xrightarrow{r \rightarrow \infty} \cos(kr - \ell \pi/2)/kr .$$

Since  $n_\ell(kr)$  is not well behaved near the origin<sup>2</sup>, if  $V(r) = 0$  everywhere then  $B_\ell$  must be chosen to be zero in order for the solution  $u_\ell$  to be valid. Thus it can be inferred that the value of  $B_\ell$  compared with  $A_\ell$  will be a measure of the strength of the potential and hence of the scattering. To make this explicit (8) can be rewritten, using the asymptotic forms above

$$u_\ell(r) \xrightarrow{r \rightarrow \infty} \frac{A_\ell}{k} \left[ \sin(kr - \frac{\ell \pi}{2}) - \frac{B_\ell}{A_\ell} \cos(kr - \frac{\ell \pi}{2}) \right]$$

and letting  $B_\ell/A_\ell = -\tan \delta_\ell$

$$u_\ell(r) \xrightarrow{r \rightarrow \infty} C_\ell \sin(kr - \frac{\ell \pi}{2} + \delta_\ell) \quad (9)$$

so that equation (6) becomes for large  $r$ , a plane wave shifted in phase from that of an unperturbed ( $V=0$ ) plane wave.  $C_\ell$  can be taken equal to one and the normalization absorbed by the expansion coefficients in equation (6).

The first term on the right hand side of (1) can be expanded as follows:

$$e^{ikr \cos \theta} = \sum_{\ell=0}^{\infty} (2\ell+1) i^\ell j_\ell(kr) P_\ell(\cos \theta) \quad (10)$$

---

<sup>2</sup> The Neumann function goes as

$$n_\ell(kr) \xrightarrow{r \rightarrow 0} \propto \frac{a}{r^{\ell+1}} + \frac{b}{r^{\ell-1}}$$



and letting  $j_\ell$  assume its asymptotic form, (6) and (1) can be equated and the result solved for  $f(\theta)$ , giving, on choosing the  $a_\ell$  so as to assure an outgoing wave,

$$f(\theta) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1) e^{i\delta_\ell} \sin \delta_\ell P_\ell(\cos \theta) \quad (11)$$

which is the usual form given for the scattering amplitude in terms of the phase shift.

Deferring the calculation of  $\delta_\ell$  to the next sections, the subject of how the above formalism must be modified in the presence of a long range coulomb potential will now be considered. Recall that the classical solution for the motion of a particle in an inverse square central force field is a hyperbola. According to an argument due to Gordon (ref. 22, p. 54), if one considers the family of classical hyperbolic trajectories with one asymptote originating at the left limit of the  $z$  axis, the surface perpendicular to these hyperbolae goes as

$$Z + a \ln k(r-z) = \text{const}$$

for large  $r$ . Thus it is as if the incident wave were initially distorted by the presence of the scattering center at infinity and its expected form would then be

$$e^{ik\{Z + a \ln k(r-z)\}}.$$

A similar argument with regard to the scattered wave leads to the form for the asymptotic wave function in the presence of a coulomb field

$$\psi(r) \xrightarrow{r \rightarrow \infty} e^{ikz + ia \ln k(r-z)} + f(\theta) \frac{e^{ikr - ia \ln 2kr}}{r}. \quad (12)$$



The coefficient  $a$  will be defined below. In solving equation (7) in the presence of the Coulomb potential one typically converts to parabolic cylindrical coordinates whereupon the Schroedinger equation becomes a version of the hypergeometric equation whose solutions are the hypergeometric functions (ref. 22, p. 57 ff). Using the asymptotic forms of the solution functions as before, equation (9) becomes, in the case of the Coulomb potential

$$u_{\ell}(r) \xrightarrow{r \rightarrow \infty} C_{\ell} \sin(kr - \frac{\ell\pi}{2} + a \ln 2kr + \eta_{\ell} + \delta_{\ell}) \quad (13)$$

where  $\delta_{\ell}$  is as defined above and

$$\eta_{\ell} = \arg \{ \Gamma(\ell+1 - ia) \} \quad (14)$$

is the phase shift at infinity due to the Coulomb potential.

Equation (11) must now be modified to account for this additional phase shift (ref. 22, p. 65 ff).

The coefficient  $a$  in (12), (13) and (14) is proportional to the charge of the scattering center. However, since the problem at hand is one in which the pure Coulomb field exists only at long range, this charge is the net charge of the ion, in this case  $(Z-1)$  where  $Z$  is the atomic number of the scattering center, and in the system of units in use  $a$  can be written

$$a = (Z-1)/k \quad (15)$$

and now  $\delta_{\ell}$  can be interpreted as the phase shift due to the departure from pure coulomb scattering at close range. It is this quantity which is of physical interest.

To summarize, it has been shown how the asymptotic form of the wave function (equations 1 or 12) can be calculated by solving the Schroedinger equation for a series of linearly independent functions





(equations 9 or 13), in other words, that the problem can be reduced to solving a series of "partial wave" equations for the various values of the angular momentum quantum number  $\ell$ . A simple kinematic argument indicates that as the energy of the incident beam is reduced the higher order terms in the expansion (6) become less important, enabling a fairly good representation of  $f(\theta)$  to be constructed using only the first few terms.

## B. THE KOHN VARIATIONAL METHOD

Before taking up the Harris method it will be worth while to briefly examine the Kohn method since it is the most widely used variational method in low energy atomic scattering and its difficulties were the motivation for Harris' development. These difficulties have been examined elsewhere [6-9] and will only be mentioned here.

The Kohn method provides an estimate of the phase shift which is "second order accurate" in the error, i.e., the error term is at least second order small. In developing the Kohn method one assumes a trial function of the form

$$\phi = \sin kr + t \cos kr + \Psi \quad (16)$$

where  $t$  is an estimate of the tangent of the phase shift and  $\Psi$  is normally a linear combination of some basis set  $\chi_i$  such that

$$\Psi = \sum_{i=1}^N a_i \chi_i \xrightarrow{r \rightarrow \infty} 0 \quad (17)$$

so that  $\phi$  is now a function of  $N+1$  parameters--the  $N$  values of  $a_i$ , and  $t$ . Let  $\Psi$  be the true wave function whose asymptotic behavior is

$$\Psi \xrightarrow{r \rightarrow \infty} \sin kr + \tan \delta \cos kr$$

$$\Psi(0) = \phi(0) = 0$$



and define the error wave function

$$\epsilon = \varphi - \Psi. \quad (18)$$

Now form the functional

$$F = \int \varphi(H-E)\varphi \, d\vec{r} \quad (19)$$

which, using the fact that  $(H-E)\Psi=0$ , can be transformed into

$$F = \int \varphi(H-E)\epsilon \, d\vec{r}.$$

Integrating twice by parts yields

$$F = -\frac{1}{2}(\varphi\nabla\epsilon - \epsilon\nabla\varphi) + \int \epsilon(H-E)\varphi \, d\vec{r}$$

and substituting (18) for  $\epsilon$  in the first two terms and for  $\varphi$  under the integral gives

$$F = \int \varphi(H-E)\varphi \, d\vec{r} = \frac{k}{2}(t - \tan\delta) + \int \epsilon(H-E)\epsilon \, d\vec{r}$$

or

$$\frac{k}{2} \tan\delta = \frac{k}{2} t - F + \int \epsilon(H-E)\epsilon \, d\vec{r} \quad (20)$$

which identity is due to Kato [24] and exhibits the nature of the error term. Now the Kohn prescription takes as its functional

$$I = \frac{k}{2} \tan\delta = \frac{k}{2} t - \int \varphi(H-E)\varphi \, d\vec{r} \quad (21)$$

and seeks its stationary value subject to the conditions

$$\frac{\partial I}{\partial t} = \frac{\partial I}{\partial a_i} = 0, \quad i=1, \dots, N.$$

The value of  $I$  thus found is the estimate of  $\tan\delta$  to second order.

## C. THE HARRIS EXPANSION METHOD

### 1. Formal Solution

It can be shown that the development of expressions for the phase shift lose no generality when the system is restricted



to one of s-waves ( $\ell=0$ ) scattered from a central potential. Therefore this restriction will be imposed on the present derivation of Harris' method [10] and the validity of its extension to atomic systems will be assumed.

With the above considerations in mind, assume a system describable by a potential  $V(r)$  and a Hamiltonian  $H$ . Construct a trial basis space using a set of  $N$  linearly independent functions  $|\chi_i\rangle$ . In this restricted space the Hamiltonian can be represented by a matrix whose elements are

$$H_{ij} = \langle \chi_i | H | \chi_j \rangle \quad (22)$$

while the inner products of the basis vectors are

$$L_{ij} = \langle \chi_i | \chi_j \rangle \quad (23)$$

Then the eigenvalue equation

$$(\underline{H} - \lambda \underline{L}) \vec{C} = 0$$

where the elements of  $\underline{H}$  and  $\underline{L}$  are as given in (22) and (23), can be solved for the  $N$  eigenvalues  $\lambda_\rho$  and corresponding eigenvectors  $\vec{C}_\rho$ , ( $\rho=1, \dots, N$ ). From the eigenvectors a new basis set is constructed (which spans the same space as the  $|\chi_i\rangle$ )

$$|\phi_\rho\rangle = \sum_{i=1}^N c_{i\rho} |\chi_i\rangle \quad (25)$$

Now if the true wave function is represented by

$$\Psi = S + tC + \Phi$$

where  $\Psi(0) = 0$

and

$$\Psi(r) \xrightarrow{r \rightarrow \infty} \sin kr + \tan \delta \cos kr = S + tC$$



(where now the identification of the terms S, t and C is clear) and if in addition  $|\Phi\rangle$  may be reasonably well represented at some energy E by  $|\xi\rangle$ , a linear combination of the  $|\varphi_\rho\rangle$ ,

$$|\xi\rangle = \sum_{\omega=1}^N b_\omega |\varphi_\omega\rangle$$

then the approximate wave function may nearly satisfy the Schroedinger equation. If this is to be the case, then in the space spanned by the  $|\varphi_\rho\rangle$  the vector

$$(H-E)|S + tC + \xi\rangle \quad (26)$$

must be the null vector, which is, of course, merely the statement of Schroedinger's equation in the restricted space of the trial functions. This condition may be satisfied if it is required that (26) have no component in the space spanned by the  $|\varphi_\rho\rangle$ , that is, that

$$\langle \varphi_\rho | (H-E) | S + tC + \xi \rangle = 0, \quad \rho=1, \dots, N. \quad (27)$$

Since the  $|\varphi_\rho\rangle$  are themselves linear combinations of the original basis set  $|\chi_i\rangle$ , the condition (27) is equivalent to requiring that (26) have no component in the space spanned by the  $|\chi_i\rangle$ . Bearing in mind that the solution sought involves finding t, an estimate of  $\tan\delta$ , note that if  $\langle \varphi_\rho | H-E | \xi \rangle$  and  $\langle \varphi_\rho | H-E | S + tC \rangle$  are separately equal to zero then (27) is satisfied and t can be immediately found. Note further that if  $E = \lambda_\rho$ , the eigenvalue found in (24) corresponding to the vector  $|\varphi_\rho\rangle$ , that then

$$\langle \varphi_\rho | (H-E) | \xi \rangle = 0 \quad (28)$$





for

$$\langle \varphi_\rho | (H-E) | \xi \rangle = \sum_{\omega=1}^N b_\omega \sum_{j=1}^N c_{j\omega} \sum_{i=1}^N \langle \chi_i | (H-\lambda_\rho) | \chi_j \rangle c_{i\rho}$$

and the third sum in this expression is merely (24) in component notation, whence

$$\sum_{i=1}^N \langle \chi_i | (H-\lambda_\rho) | \chi_j \rangle c_{i\rho} = 0, \quad j=1, \dots, N$$

irrespective of the value of  $\omega$ . Hence (28) is satisfied and it follows immediately from (27) that

$$\tan \delta = t = - \frac{\langle \varphi_\rho | (H-E_\rho) | S \rangle}{\langle \varphi_\rho | (H-E_\rho) | C \rangle} \quad (29)$$

and the problem is formally solved. Finally as the size of the basis set  $|\chi_i\rangle$  is increased (i.e., approaches a complete set of quadratically integrable functions)  $|\xi\rangle$  should more closely approach  $|\hat{\xi}\rangle$  and  $t$  should converge to the correct result.

Kolker [25] has shown that the Harris method can be formulated as a variational principle and that under certain conditions it can be combined with the Kohn method to give a minimum principle. The advantage of the Harris method is principally computational, in that no integrals of the form  $\langle S | (H-E) | C \rangle$  need be evaluated. However the contribution of these integrals is needed to provide the second order correction to the estimate of  $\tan \delta$  in variational methods dependent upon the Kato identity (20), so it can be seen that the Harris method is necessarily less accurate than the Kohn method, as was found by Nesbet [8]. It remains true, however, that the correction term can be made arbitrarily small by



increasing the size of the trial basis set, for as this set approaches completeness, the error must approach zero.

## 2. Application to Atomic Scattering

In applying the Harris formalism to the problem of atomic scattering the Hamiltonian is written as follows

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \quad (30)$$

where the subscripts refer to the individual electrons,  $Z$  is the atomic number of the scattering atom and  $r_{12} = |\vec{r}_1 - \vec{r}_2|$  is the inter-electron distance. The zero of total energy in this system occurs with all three particles at rest and separated from one another by an infinite distance. The trial basis set is taken as the Hylleraas-type functions [20]

$$\chi_i = \left( r_1^n r_2^\ell + r_1^\ell r_2^n \right) r_{12}^m e^{-\frac{\alpha}{2}(r_1 + r_2)} \quad (31)$$

where  $n$ ,  $\ell$  and  $m$  are integers, chosen subject to the constraint

$$n + \ell + m \leq M, \quad (M=1,2,\dots) \quad (32)$$

and  $\alpha$  is a variable parameter.

This form of the wave function allows for electron exchange, i.e., the interchange of roles between bound and free during the scattering process, and enables the wave function to be properly symmetrized when the electron spins are anti-parallel (spin = 0, or "singlet" state) or anti-symmetrized when the spins are parallel (spin = 1, or "triplet" state) thus satisfying the requirements of the Pauli principle [26,27]. This is the only way the spin enters the problem and so once the symmetry of the wave function is properly chosen no further concern need be taken with the spin



coordinates of the electrons. Inclusion of the  $r_{12}$  term in the potential and in the wave function takes account of the induced polarization of the atom arising from the repulsion felt by the bound electron as the incident electron approaches. Finally, the exponential term forces the functions to zero as  $r_1$  or  $r_2$  increases so that all boundary conditions required for these functions in the last section are met. As will be seen below the parameter  $\alpha$  is varied by inspection so as to optimize the results obtained.

The number of functions in the basis set is found by taking all possible combinations of  $n, \ell, m$  subject to the constraint (32) for a given  $M$ , and eliminating all terms which duplicate the function or require it to be identically zero irrespective of the choice of sign. The results for  $1 \leq M \leq 8$  are shown in Table I.

M	No. terms in basis set	
	Singlet	Triplet
1	3	1
2	7	3
3	13	7
4	22	13
5	34	22
6	50	34
7	70	50
8	95	70

Table I. Basis set size for various  $M$ .

The choice of coordinate system is of importance in simplifying the computational details. For the present computation the optimum choice seemed to be the one in which the principle coordinates are the radius vectors of the two electrons and the angle formed by the radius vectors. The six coordinates governing motion of the center of mass and orientation of the system in space



are cyclic, and the Hamiltonian becomes [28]

$$- \frac{1}{2} \left[ \frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1} \frac{\partial}{\partial r_1} + \frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2} \frac{\partial}{\partial r_2} + \left( \frac{1}{r_1^2} + \frac{1}{r_2^2} \right) \sin \theta_{12} \frac{\partial}{\partial \theta_{12}} \left( \sin \theta_{12} \frac{\partial}{\partial \theta_{12}} \right) \right] \\ - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \quad (33)$$

where  $r_{12} = (r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta_{12})^{\frac{1}{2}}$  by the law of cosines, and the volume element for integrals in this system is

$$d\vec{r}_1 d\vec{r}_2 = 8\pi^2 r_1^2 dr_1 r_2^2 dr_2 \sin \theta_{12} d\theta_{12} . \quad (34)$$

The advantage of this system is that all of the integrals arising from forming the matrices  $\underline{H}$  and  $\underline{L}$  (equations 22-24) can be done exactly, while those arising from  $\langle \varphi | (H-E) | S+tC \rangle$  can be done exactly in the case of hydrogen and reduce to single integrals which then can be done numerically in the case of helium ions.

Because the electrons are identical and thus formally indistinguishable it is not necessary to integrate over the entire first quadrant of the  $r_1, r_2$  plane. It is sufficient to cover only the region  $r_1 \geq r_2$  [29]. To see why this is true one must examine the integrals generated in forming  $H_{ij}$  and  $L_{ij}$  using (31) and (33). Carrying out the indicated operations gives rise to 52 terms for each  $H_{ij}$  and four terms for each  $L_{ij}$ . Each term consists of an integral of the form

$$A(\nu, \lambda, \mu) = \int d\vec{r}_1 d\vec{r}_2 e^{-\alpha(r_1+r_2)} r_1^{\nu-2} r_2^{\lambda-2} r_{12}^{\mu-2} \quad (35)$$

or

$$B(\nu, \lambda, \mu) = \int d\vec{r}_1 d\vec{r}_2 e^{-\alpha(r_1+r_2)} r_1^{\nu-2} r_2^{\lambda-2} r_{12}^{\mu-2} \cos \theta_{12} . \quad (36)$$





The complete expressions for  $H_{ij}$  and  $L_{ij}$  are given in Appendix A.

Examination of the terms comprising  $H_{ij}$  and  $L_{ij}$  indicates that every term involving  $A(v, \lambda, 0)$  and  $B(v, \lambda, 0)$  always has a coefficient of zero. Since the angular integration of  $B(v, \lambda, 2)$  vanishes,  $B(v, \lambda, 2) = 0$ , so using the recursion relations proved in Appendix B it is sufficient to explicitly evaluate only the  $A(v, \lambda, 2)$  in order to find all the terms required to generate the  $H_{il}$  and  $L_{ij}$ .

Setting  $\mu = 2$  in (35) and performing the angular integration over the range 0 to  $\pi$ , gives, in terms of the integration region outlined in Figure 1 below and the volume element (34)

$$A(v, \lambda, 2) = 16 \pi^2 \int_0^\infty r_1^v e^{-\alpha r_1} dr_1 \int_0^{r_1} r_2^\lambda e^{-\alpha r_2} dr_2. \quad (37)$$

Inspection of  $H_{ij}$  shows that for each term of the form (37) there is another of the form

$$A(\lambda, v, 2) = 16 \pi^2 \int_0^\infty dr_1 r_1^\lambda e^{-\alpha r_1} \int_0^{r_1} dr_2 r_2^v e^{-\alpha r_2} \quad (38)$$

which is the mathematical equivalent of integrating (37) in the region  $r_2 \geq r_1$  as can be seen immediately by making the variable change  $r_1 \rightleftharpoons r_2$  in (38). Thus as a result of the exchange of particles possible because the electrons are identical, the integrals (37) are sufficient to cover the entire quadrant. This argument is extended below to the integrals arising in  $\langle \varphi | (H-E) | S+tC \rangle$ .

Equation (37) may be integrated directly, giving

$$A(v, \lambda, 2) = \frac{16 \pi^2 \lambda!}{\alpha^{v+\lambda+2}} \left[ v! - \frac{1}{2} \sum_{i=0}^{\lambda} \frac{(\lambda-i)!}{2^{v+\lambda-1} (\lambda-i)!} \right]. \quad (39)$$



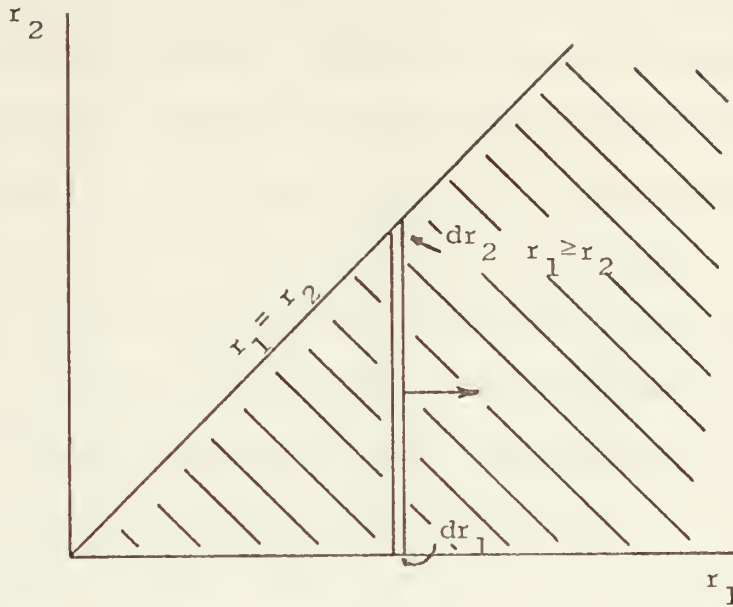


Figure 1. Integration Region for  $A(v, \lambda, 2)$ .

The factor  $16\pi^2$  appears in every integral; it can be dropped from the calculation since it will merely give rise to the same constant factor in both  $\underline{H}$  and  $\underline{L}$  and will not affect the solution of the problem. Because of the way the recursion relations are structured the factor  $1/\alpha$  always occurs in the form  $1/\alpha^{v+\lambda+\mu}$  and thus can be factored out of the integration and incorporated into the coefficient of each term in the expression for  $H_{ij}$  and  $L_{ij}$ . Since this is the only way the parameter  $\alpha$  enters these integrations, evaluating all the integrals need only be done once at the beginning of the calculation for a given basis and the values thus found can be used over again as  $\alpha$  is varied.

Unfortunately a similar simplification is not available with the integrals from  $\langle \varphi_\rho | (H-E) | S+tC \rangle$ . However as will be seen only a relatively few integrals must be done numerically for each value of  $\alpha$  and  $k$  and so the time required to complete the numerical



integration (which dominated the time required to evaluate the helium ion phase shifts in all but the largest basis sets) was kept within reasonable bounds. Since the present calculation is concerned only with the s partial wave ( $\ell=0$ ) further discussion will assume  $\ell$  has been set equal to zero in all equations of the form (9), (13) or (14). Furthermore, since the proper form for hydrogen results if (13) is taken as the asymptotic form of the wave function and  $Z$  is set equal to one in (15), the remainder of the development will be concerned exclusively with establishing the Harris method in the presence of a long range Coulomb field.

Bearing these comments in mind, note that as  $r$  goes to zero (13) does not behave as well as one would like. Because of the presence of the logarithmic term in the argument of the sine, as  $r$  approaches zero the interval between zeroes of the function approaches zero and  $u(r)$  does not approach a definite limit. To force  $u(r)$  to zero a factor is normally chosen which goes to zero fast enough as  $r$  goes to zero to override the effects of any singularity which may occur, and goes to unity as  $r$  gets large in order not to affect the asymptotic behavior of the function. For the present calculation the factor was chosen to be  $(1-\exp(-\alpha r/2))^3$ . This choice was made to insure that  $u(r)$  would go to zero fast enough that its oscillatory behavior near the origin would not affect the accuracy of the numerical integrations involving the asymptotic part of the wave functions.

With these preliminaries aside, the form chosen for the asymptotic part of the wave function may now be presented:



$$\begin{aligned}
S+tC = & e^{-Zr_1} \left(1 - e^{-\frac{\alpha}{2} r_2}\right) 3 \left[ \sin\left(kr_2 + \frac{Z-1}{k} \ln 2kr_2 + \eta\right) \right. \\
& + \tan\delta \cos\left(kr_2 + \frac{Z-1}{k} \ln 2kr_2 + \eta\right) \left. \right] / r_2 \\
& \pm e^{-Zr_2} \left(1 - e^{-\frac{\alpha}{2} r_1}\right) 3 \left[ \sin\left(kr_1 + \frac{Z-1}{k} \ln 2kr_1 + \eta\right) \right. \\
& + \tan\delta \cos\left(kr_1 + \frac{Z-1}{k} \ln 2kr_1 + \eta\right) \left. \right] / r_1
\end{aligned} \tag{40}$$

where

$$\eta = \arg \left\{ \Gamma\left(1 - i \frac{Z-1}{k}\right) \right\} . \tag{41}$$

Evaluation of the complex Gamma functions is discussed in Appendix D. Normalization factors in (40) have been suppressed because they do not affect the calculation, cancelling when  $t$  is evaluated.

Following the prescription outlined in section 1, the estimate of  $\tan\delta$  is evaluated from the ratio of the integrals  $\langle \varphi_\rho | (H-E) | S \rangle$  and  $\langle \varphi_\rho | (H-E) | C \rangle$  at the energy  $E_\rho$  found by solving (24). Since the functions  $(H-E)|\chi_i\rangle$  have been previously evaluated in solving (22) and (23), considerable simplification is achieved by taking advantage of the fact that  $H$  is a hermitian operator and solving instead the equivalent integrals

$$\sum_{i=1}^N c_{i\rho} \langle S | (H-E_\rho) | \chi_i \rangle \tag{42}$$

and

$$\sum_{i=1}^N c_{i\rho} \langle C | (H-E_\rho) | \chi_i \rangle \tag{43}$$

whence  $t$  is found from the negative ratio of (42) to (43). Note again that  $\delta$  measures only the departure from pure Coulomb





scattering arising in the region close to the target where the three particles in the system must be treated explicitly.

Carrying out the indicated algebra one finds that  $\langle S | (H-E) | \chi \rangle$  has 52 terms constructed of integrals of the form

$$A_1(\nu, \lambda, \mu) = \int r_1^{\nu-2} r_2^{\lambda-2} r_{12}^{\mu-2} e^{-(Z+\frac{\alpha}{2})r_1} e^{-\frac{\alpha}{2}r_2} \left(1 - e^{-\frac{\alpha}{2}r_2}\right)^3 \times \\ \sin(kr_2 + \frac{Z-1}{k} \ln 2kr_2 + \eta) d\vec{r}_1 d\vec{r}_2 \quad (44)$$

$$A_2(\nu, \lambda, \mu) = \int r_1^{\nu-2} r_2^{\lambda-2} r_{12}^{\mu-2} e^{-(Z+\frac{\alpha}{2})r_2} e^{-\frac{\alpha}{2}r_1} \left(1 - e^{-\frac{\alpha}{2}r_1}\right)^3 \times \\ \sin(kr_1 + \frac{Z-1}{k} \ln 2kr_1 + \eta) d\vec{r}_1 d\vec{r}_2 \quad (45)$$

$$B_1(\nu, \lambda, \mu) = \int r_1^{\nu-2} r_2^{\lambda-2} r_{12}^{\mu-2} e^{-(Z+\frac{\alpha}{2})r_1} e^{-\frac{\alpha}{2}r_2} \left(1 - e^{-\frac{\alpha}{2}r_2}\right)^3 \times \\ \sin(kr_2 + \frac{Z-1}{k} \ln 2kr_2 + \eta) \cos\theta_{12} d\vec{r}_1 d\vec{r}_2 \quad (46)$$

$$B_2(\nu, \lambda, \mu) = \int r_1^{\nu-2} r_2^{\lambda-2} r_{12}^{\mu-2} e^{-(Z+\frac{\alpha}{2})r_2} e^{-\frac{\alpha}{2}r_1} \left(1 - e^{-\frac{\alpha}{2}r_1}\right)^3 \times \\ \sin(kr_1 + \frac{Z-1}{k} \ln 2kr_1 + \eta) \cos\theta_{12} d\vec{r}_1 d\vec{r}_2 \quad (47)$$

Four similar integrals with  $\cos(kr + \dots)$  replacing the sine terms in (44) - (47) arise in evaluating  $\langle C | (H-E) | \chi \rangle$  and are designated  $A_3$ ,  $A_4$ ,  $B_3$ , and  $B_4$ , respectively. Note that all these integrals are of the same form as those in Appendix B Section 1 and hence the same recursion relations may be applied.



As with the integrals of equation (34) the evaluation of (44) - (47) starts with the case  $\mu = 2$  and as before, the angular integration yields  $B_1(\nu, \lambda, 2) = B_2(\nu, \lambda, 2) = 0$  and introduces a factor 2 in the coefficient of  $A_1(\nu, \lambda, 2)$  and  $A_2(\nu, \lambda, 2)$ . Also as with the  $A(\nu, \lambda, 2)$ , terms of the form  $A_1(\nu, \lambda, 2)$  and  $A_2(\nu, \lambda, 2)$  always exist together and thus satisfy the requirements that allow the integration to proceed over  $r_1 \geq r_2$  only, as illustrated in Figure 1.

Starting first with  $A_1(\nu, \lambda, 2)$ , after angular integration

$$A_1(\nu, \lambda, 2) = 16\pi^2 \int_0^\infty dr_1 r_1^\nu e^{-(Z + \frac{\alpha}{2})r_1} \int_0^{r_1} dr_2 r_2^\lambda e^{-\frac{\alpha}{2}r_2} \left(1 - e^{-\frac{\alpha}{2}r_2}\right)^3 \times$$

$$\sin(kr_2 + \frac{Z-1}{k} \ln 2kr_2 + \eta).$$

Now referring to Figure 2, note that the order of integration can be reversed by choosing the elements of area  $dr_1 dr_2$  as indicated while the same region is covered. With this change  $A_1(\nu, \lambda, 2)$  becomes

$$A_1(\nu, \lambda, 2) = 16\pi^2 \int_0^\infty dr_2 r_2^\lambda e^{-\frac{\alpha}{2}r_2} \left(1 - e^{-\frac{\alpha}{2}r_2}\right)^3 \times$$

$$\sin(kr_2 + \frac{Z-1}{k} \ln 2kr_2 + \eta) \int_{r_2}^\infty dr_1 r_1^\nu e^{-(Z + \frac{\alpha}{2})r_1}$$

and now the integral over  $r_1$  can be done giving

$$A_1(\nu, \lambda, 2) = \frac{32\pi^2 \nu!}{2Z + \alpha} \sum_{i=0}^{\nu} \frac{1}{(\nu-1)!(Z + \frac{\alpha}{2})^i} \int_0^\infty dr_2 r_2^{\nu+\lambda-i} e^{-(Z+\alpha)r_2} \left(1 - e^{-\frac{\alpha}{2}r_2}\right)^3$$

$$\times \sin(kr_2 + \frac{Z-1}{k} \ln 2kr_2 + \eta)$$



Finally, making the variable change  $x = (Z + d)r_2$

$$A_1(\nu, \lambda, 2) = \frac{32\pi^2 \nu!}{(2Z+\alpha)(Z+\alpha)^{\nu+\lambda+1}} \sum_{i=0}^{\nu} \left( \frac{2Z+2\alpha}{2Z+\alpha} \right)^i \frac{1}{(\nu-i)!} I_1(\nu+\lambda-i) \quad (48)$$

where

$$I_1(\gamma) = \int_0^{\infty} e^{-x} x^{\gamma} \left( 1 - e^{-\frac{\alpha x}{2(Z+\alpha)}} \right)^3 \sin\left( \frac{kx}{Z+\alpha} + \frac{Z-1}{k} \ln \frac{2kx}{Z+\alpha} + \eta \right) dx \quad (49)$$

when  $Z = 2$  ( $\text{He}^+$ ), equation (49) must be evaluated numerically. However when  $Z = 1, \eta = 0$  and the integral reduces to a standard form [30]. Numerical evaluation of (49) is discussed in Appendix D.

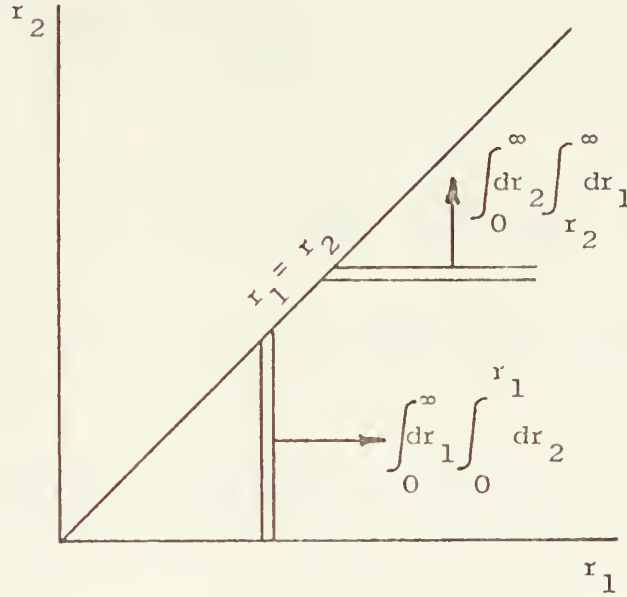


Figure 2. Interchanging the  $r_1$  and  $r_2$  Integration.

Proceeding now to the evaluation of  $A_2(\nu, \lambda, 2)$ , note that the  $r_2$  integration may be done directly and that evaluating it at the upper limit ( $r_1$ ) gives the same function of  $r_1$  as did the evaluation of the  $r_1$  integration at the lower limit ( $r_2$ ) in the evaluation of  $A_1(\nu, \lambda, 2)$  but with  $\nu$  and  $\lambda$  interchanged:



$$A_2(\nu, \lambda, 2) = \frac{32\pi^2 \lambda!}{2Z+\alpha} \left\{ \left( \frac{2}{2Z+\alpha} \right)^\lambda \int_0^\infty dr_1 \left( 1 - e^{-\frac{\alpha}{2} r_1} \right)^3 e^{-\frac{\alpha}{2} r_1} r_1^\nu \sin\left(kr_1 + \frac{Z-1}{k} \ln 2kr_1 + \eta\right) \right. \\ \left. - \sum_{i=0}^{\nu} \left( \frac{2}{2Z+\alpha} \right)^i \frac{1}{(\lambda-i)!} \int_0^\infty dr_1 \left( 1 - e^{-\frac{\alpha}{2} r_1} \right)^3 e^{-(Z+\alpha)r_1} r_1^{\nu+\lambda-i} \sin\left(kr_1 + \frac{Z-1}{k} \ln 2kr_1 + \eta\right) \right\}$$

Making the variable change  $x = \alpha r_1/2$  in the first term and  $x = (Z+\alpha)r_1$  in the remaining terms, and recognizing that the summation is in fact  $A_1(\lambda, \nu, 2)$  gives

$$A_2(\nu, \lambda, 2) = \frac{32\pi^2 \lambda!}{(2Z+\alpha)\alpha^{\nu+1}} \frac{2^{\nu+\lambda+1}}{(2Z+\alpha)^\lambda} I_s(\nu) - A_1(\lambda, \nu, 2) \quad (50)$$

where

$$I_s(\gamma) = \int_0^\infty e^{-x} x^\gamma (1-e^{-x})^3 \sin\left(\frac{2kx}{\alpha} + \frac{Z-1}{k} \ln \frac{4kx}{\alpha} + \eta\right) dx. \quad (51)$$

Now since  $A_1(\nu, \lambda, 2)$  and  $A_2(\lambda, \nu, 2)$  always occur together it is convenient to define

$$A_s(\lambda, \nu, 2) = A_1(\nu, \lambda, 2) + A_2(\lambda, \nu, 2) \quad (52)$$

and similarly

$$A_s(\lambda, \nu, \mu) = A_1(\nu, \lambda, \mu) + A_2(\lambda, \nu, \mu) \quad (53a)$$

$$B_s(\lambda, \nu, \mu) = B_1(\nu, \lambda, \mu) + B_2(\lambda, \nu, \mu) \quad (53b)$$

$$A_c(\lambda, \nu, \mu) = A_3(\nu, \lambda, \mu) + A_4(\lambda, \nu, \mu) \quad (53c)$$

$$B_c(\lambda, \nu, \mu) = B_3(\nu, \lambda, \mu) + B_4(\lambda, \nu, \mu) \quad (53d)$$

where (53a) and (53b) arise in evaluating  $\langle S | (H-E) | \chi \rangle$  and (53c) and (53d) arise in evaluating  $\langle C | (H-E) | \chi \rangle$  and the number of terms in each is now reduced to 26. Unfortunately, explicit expressions for  $A_1(\nu, \lambda, 2)$  and  $A_3(\nu, \lambda, 2)$  are required in order to evaluate  $A_s(\nu, \lambda, 1)$ ,





$B_s(v, \lambda, 1)$ ,  $A_c(v, \lambda, 1)$  and  $B_c(v, \lambda, 1)$ , respectively so the reduction in labor is not so great as it might appear. Note that the factor  $32\pi^2/(2Z+\alpha)$  is common to every term, so it may be dropped from the calculation.

### 3. Summary of the Harris Method

To summarize the Harris prescription as it applies to atomic scattering, the computational scheme is as follows:

a. For the given basis set size evaluate the required "close-in" integrals from

$$A(v, \lambda, 2) = \lambda! \left\{ v! - \frac{1}{2^{v+\lambda+1}} \sum_{i=0}^{\lambda} \frac{2^i (\lambda+v-i)!}{(\lambda-i)!} \right\} \quad (54)$$

b. Evaluate the required  $A(v, \lambda, \mu)$  and  $B(v, \lambda, \mu)$  using the recursion relations of Appendix B.

c. For a given  $\alpha$ , evaluate  $H_{ij}$  and  $L_{ij}$  using the expressions in Appendix A. Note that each A and B must be divided by  $\alpha^{v+\lambda+\mu}$  to give the correct result.

d. Solve the eigenvalue problem (24) for the eigenvalues  $E_\rho$  and corresponding eigenvectors  $\vec{c}_\rho$ .

e. Find an appropriate incident electron momentum from the expression

$$k_\rho^2 = 2E_\rho + Z^2 \quad (55)$$

where  $-Z^2$  gives the ground state energy of the scattering center in rydbergs (1 ryd = 13.6 eV).

f. For this value of  $k$  and the previously assigned value of  $\alpha$ , evaluate (numerically if necessary)  $I_1$ ,  $I_s$ ,  $I_3$  and  $I_c$  for the required values of the index  $\gamma$  using (49) and (51) for  $I_1$  and  $I_s$  and



$$I_3(\gamma) = \int_0^\infty e^{-x} x^\gamma \left(1 - e^{-\frac{\alpha x}{2(Z+\alpha)}}\right)^3 \cos\left(\frac{kx}{Z+\alpha} + \frac{Z-1}{k} \ln \frac{2kx}{Z+\alpha} + \eta\right) dx \quad (56)$$

and

$$I_c(\gamma) = \int_0^\infty e^{-x} x^\gamma (1 - e^{-x})^3 \cos\left(\frac{2kx}{\alpha} + \frac{Z-1}{k} \ln \frac{4kx}{\alpha} + \eta\right) dx \quad (57)$$

g. Using these values, evaluate the required terms of  $A_s$ ,  $A_1$ ,  $A_c$  and  $A_3$  for  $\mu = 2$  using (48) and (50).

h. Using the recursion relations in Appendix B evaluate the remaining required terms of  $A_s$ ,  $B_s$ ,  $A_c$  and  $B_c$ .

i. Evaluate the  $\langle S | (H-E) | \chi_i \rangle$  and  $\langle C | (H-E) | \chi_i \rangle$  using the expression in Appendix A and form  $\sum_{i=1}^N c_{i\rho} \langle S | (H-E) | \chi_i \rangle$  and  $\sum_{i=1}^N c_{i\rho} \langle C | (H-E) | \chi_i \rangle$ .

j. Finally the negative quotient of the two sums above is  $\tan\delta(k_\rho)$ , the desired result, and repetition of the above step for various  $\alpha$  normally permits the entire desired range of  $k_\rho$  to be covered.



### III. RESULTS AND DISCUSSION

The calculations reported in this section were performed in double-precision (16 figures) arithmetic on the IBM 360/67 computer of the Naval Postgraduate School Computer Facility. The programming language was Fortran IV and the H-level compiler was used. The subroutines used to factor the matrix  $\underline{L}$  and invert  $\underline{U}$  and to solve the eigenvalue problem, and the 32-point Gauss-Legendre quadrature subroutine, as well as several auxiliary subroutines were furnished by the source library of the Computer Facility.

The principal program was, of course, written to evaluate the phase shifts. This program and its required subroutines are reproduced following the appendices. In addition it was found convenient to have available modifications of the main program which solved only the eigenvalue problem, giving in one case the values of the incident electron momenta in the elastic scattering range and in the other the calculated energy levels of the bound state system. Since the scheme adopted for checking the eigenvalues and eigenvectors was rather time consuming and involved a rather large quantity of printed output, it was done on only selected matrices and then only in the supplementary programs. The modification of the phase shift program to perform these supplementary functions is obvious and the programs so modified are not reproduced here. Several features were built into the programs to permit the maximum flexibility with the minimum of internal changes and as it finally evolved only the storage capacity within the program had to be



changed, depending on the size of the basis set to be used. All other options were controlled by data inputs from external devices.

The results for e-H scattering will be presented first, followed in part B by the e-He<sup>+</sup> results. Comparison with the results of other calculations will be made where appropriate. The results will be presented in the following order: (i) phase shifts for singlet and triplet scattering; (ii) location of resonance levels; and (iii) bound state energy levels from the eigenvalue problem (see Appendix C).

## A. ELECTRON-HYDROGEN SCATTERING

### 1. Phase Shifts

Singlet and triplet phase shifts were calculated for basis sets from  $N = 22$  elements ( $M = 4$ , singlet;  $M = 5$ , triplet) to  $N = 70$  elements ( $M = 7$ , singlet;  $M = 8$ , triplet). Although the program had built into it the capability of calculating phase shifts for the 95-element basis set ( $M = 8$ , singlet) the eigenvalue problem began to show signs of instability at this size and the computer time required to find eigenvalues and eigenvectors became unacceptably long (8-10 minutes per matrix), permitting no more than testing the program at this level. In addition the storage area required for such programs approached the limit available on the computer.

Preliminary to calculating the phase shifts, equation (24) was solved for a wide range of values of the non-linear parameter  $\alpha$  and the resulting values of incident electron wave number were plotted as a function of  $\alpha$ . As expected, the eigenvalues fell into





clearly discernable trajectories whose evolution as  $N$  was increased was easily traceable, at least in those regions where the eigenvalues were sparse. Figure 3 shows such a plot for the singlet states of hydrogen with  $N = 70$ .

This plot clearly illustrates a major disadvantage of the Harris method, which has been alluded to by others [13,25] in the context of the inconvenience of being unable to pick the scattering energy without the expenditure of considerable labor. The disadvantage seems to be of a more fundamental nature, however. While coverage of the entire energy range is certainly possible, at least in most cases (it was not possible with the basis sets used to reach zero energy in the e-H triplet case), sufficient points at any given value of  $k$  are not always available to permit the sort of investigation of convergence rate that characterized the analyses of Schwartz [12] and Armstead [31]. Furthermore in those regions where few eigenvalues exist there is no guarantee that they will exist for an optimum value of  $\alpha$ . Schwartz has indicated that the useable range of  $\alpha$  was between about 0.8 and 4.0 in his calculation, and this generally proved true in the present case also. Reference to Figure 3 shows that even in the largest basis set used the value of  $\alpha$  for the only trajectory passing  $k = 0.1$  is around 5.0, just outside this range. In this region, increasing  $N$  is not likely to produce additional eigenvalues at which to solve the phase shift problem, for as is shown in Appendix C, the eigenvalues result from a Rayleigh-Ritz variational calculation of the energy levels on the two-electron bound system (see part 3 of this section) and hence the eigenvalue trajectories shown in Figure 3 represent approximations



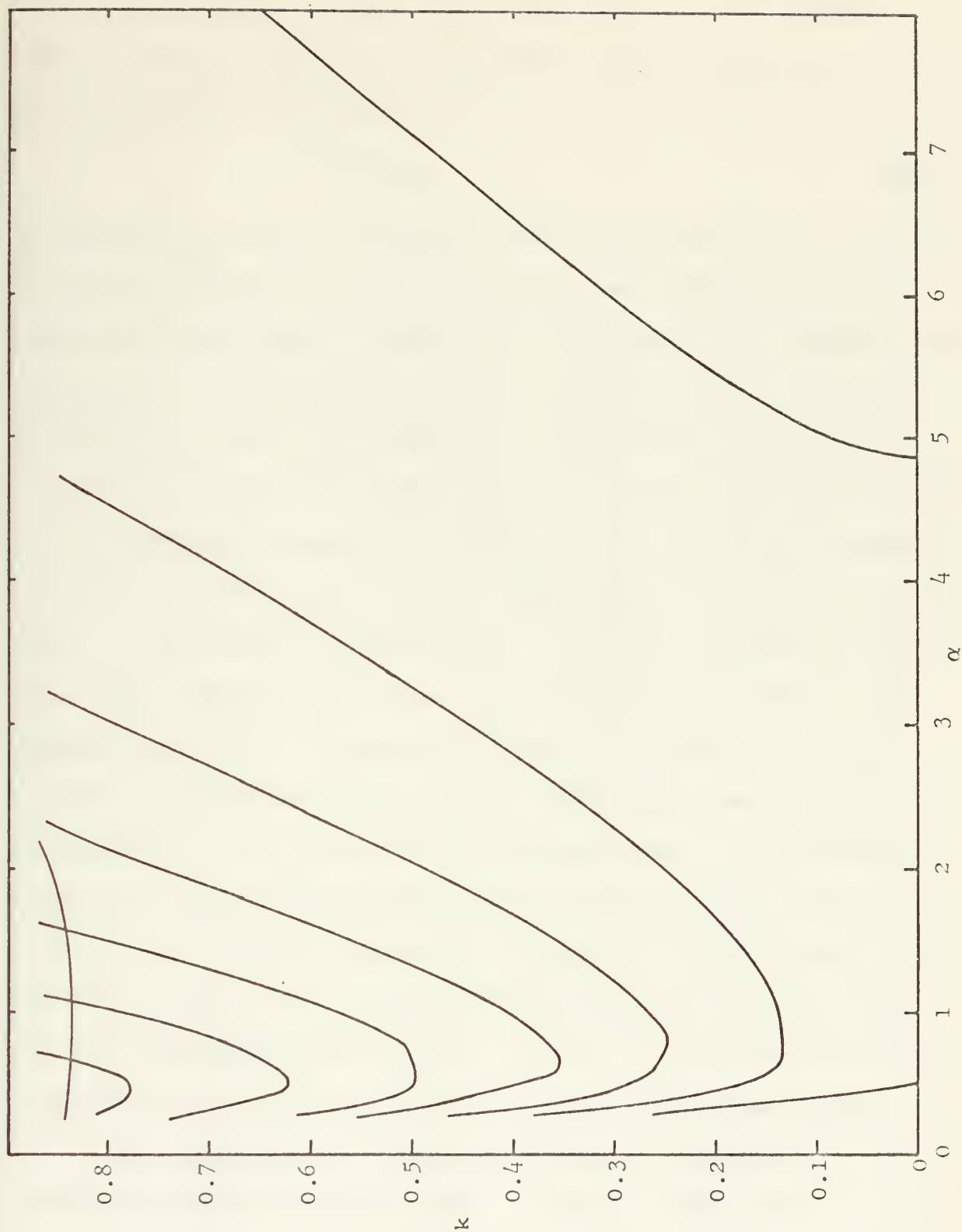


Figure 3. Eigenvalue Trajectories for Singlet e-H System  $N = 70$ .



to the various energy levels of  $H^-$  for a given  $\alpha$ . Although the scale is not the energy scale one usually associates with such plots the relationship between the two is

$$k^2 = 2E + 1 \quad (58)$$

in the case of hydrogen, where  $E$  is given in atomic units (27.2 eV). In such calculations, as  $N$  increases the lowest lying trajectories become quite good approximations to the energies of the lowest lying eigenstates of the bound system [32] after which further increase in  $N$  will give rise to no additional trajectories in that region. In fact the situation is likely to get worse from the point of view of the scattering calculation, since as  $N$  is increased the minima in the trajectories become broader, approaching horizontal straight lines as completeness is approached. Consider an incident electron wave number near but above that corresponding to the highest well defined energy level of the bound system for a given  $N$ . As  $N$  is further increased the values of  $\alpha$  for which such a wave number is an eigenstate of the system will be pushed closer to, and perhaps beyond, the limits of the range in  $\alpha$  for which reliable results can be expected. Figure 4 illustrates this behavior for a typical eigenvalue trajectory. As  $N$  is increased the curve becomes broader and its minimum approaches a limit. For  $N > 70$  the minimum probably will not decrease appreciably but the curve will become broader.

One might conclude that in an energy region which is rich in eigenvalues the situation ought to improve. That such is not always the case can be seen by examining Figures 5 and 6, showing singlet phase shifts for  $k = 0.4$  and  $0.8$  plotted as a function of  $\alpha$ . It must be noted that the lines connecting the points arising from



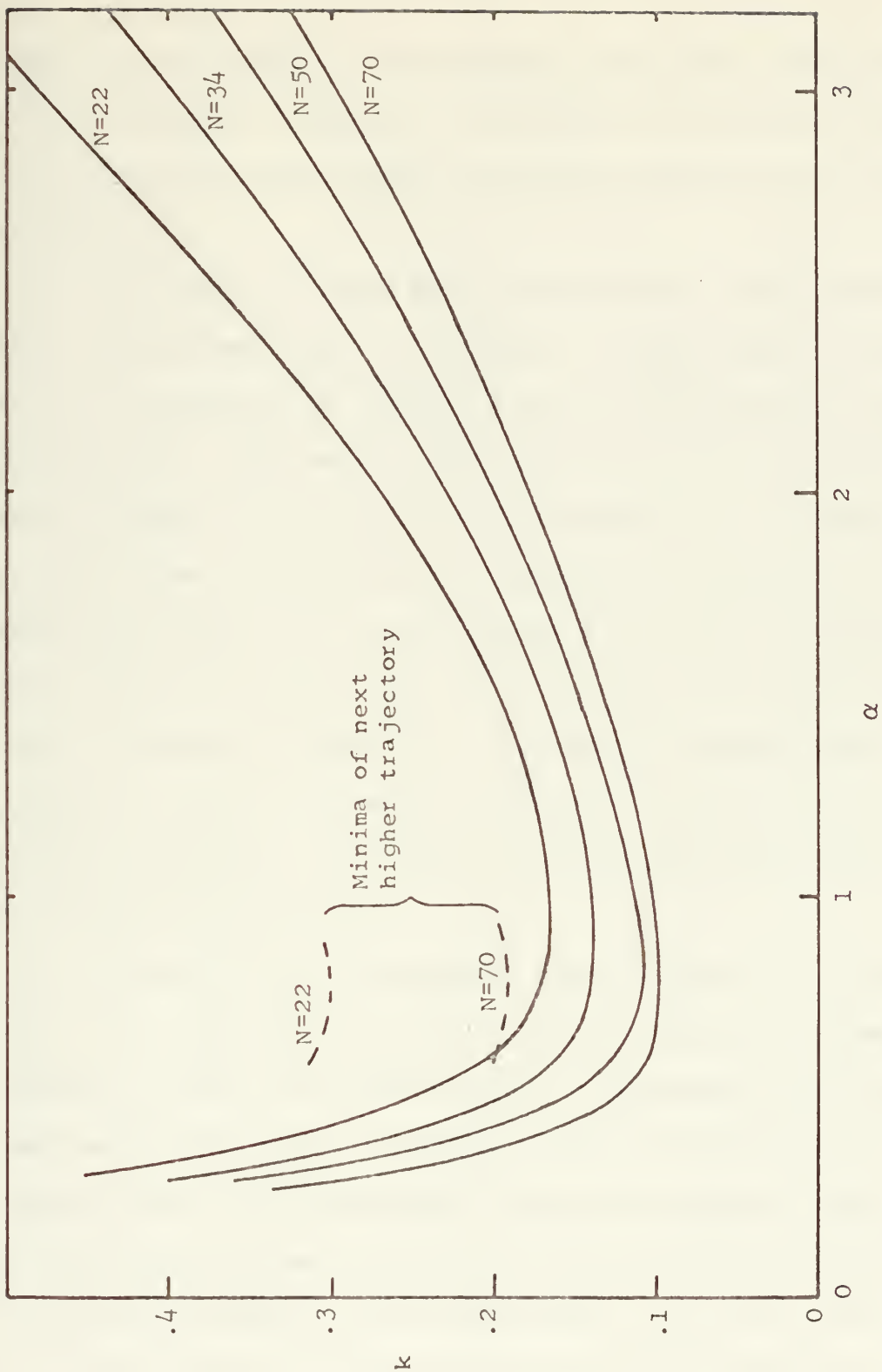


Figure 4. Typical Evolution of One Eigenvalue Trajectory as  $N$  is Increased.





the calculations for a given basis set are just that and no more. They have no physical or mathematical meaning, for the points plotted represent a complete collection of the possible values to be found at a given energy (possibly neglecting one or two at small  $\alpha$ ).

In Figure 5, while the "curves" of all basis sets have clear cut minima, there is no clearly defined trend as the basis set size increases, as Schwartz and Armstead observed in their Kohn calculations. This may be due to numerical errors which accumulate more rapidly as the basis set is increased in size, however as will be seen below the ambiguity is considerably reduced in the triplet case which leads one to conclude that this error is probably small. Note however that the range of  $\alpha$  over which the phase shift is nearly constant is greatest for the case  $N = 70$  and hence the minimum of that curve has been selected as the most probable value in this calculation. The rather large error indications in Table II reflect this situation.

Referring now to Figure 6, note that while the minimum of the  $N = 70$  curve is at  $\delta = 0.761$ , there is a plateau forming around  $\delta = 0.886$ . For this value of  $k$  increasing  $N$  may well bring improved results since the minima of more trajectories may be expected to move into the region, however the ambiguity will remain if the plateau becomes broader and stable in value. A similar structure is evident in the calculations for  $k = 0.7$  and  $0.6$  as well. It is interesting to note that these plateaus correspond to the values for the phase shift given by Schwartz and the difference between these plateaus and the minima of the curves increases with increasing  $k$  until at  $k = 0.866$  the difference is in excess of 10%.



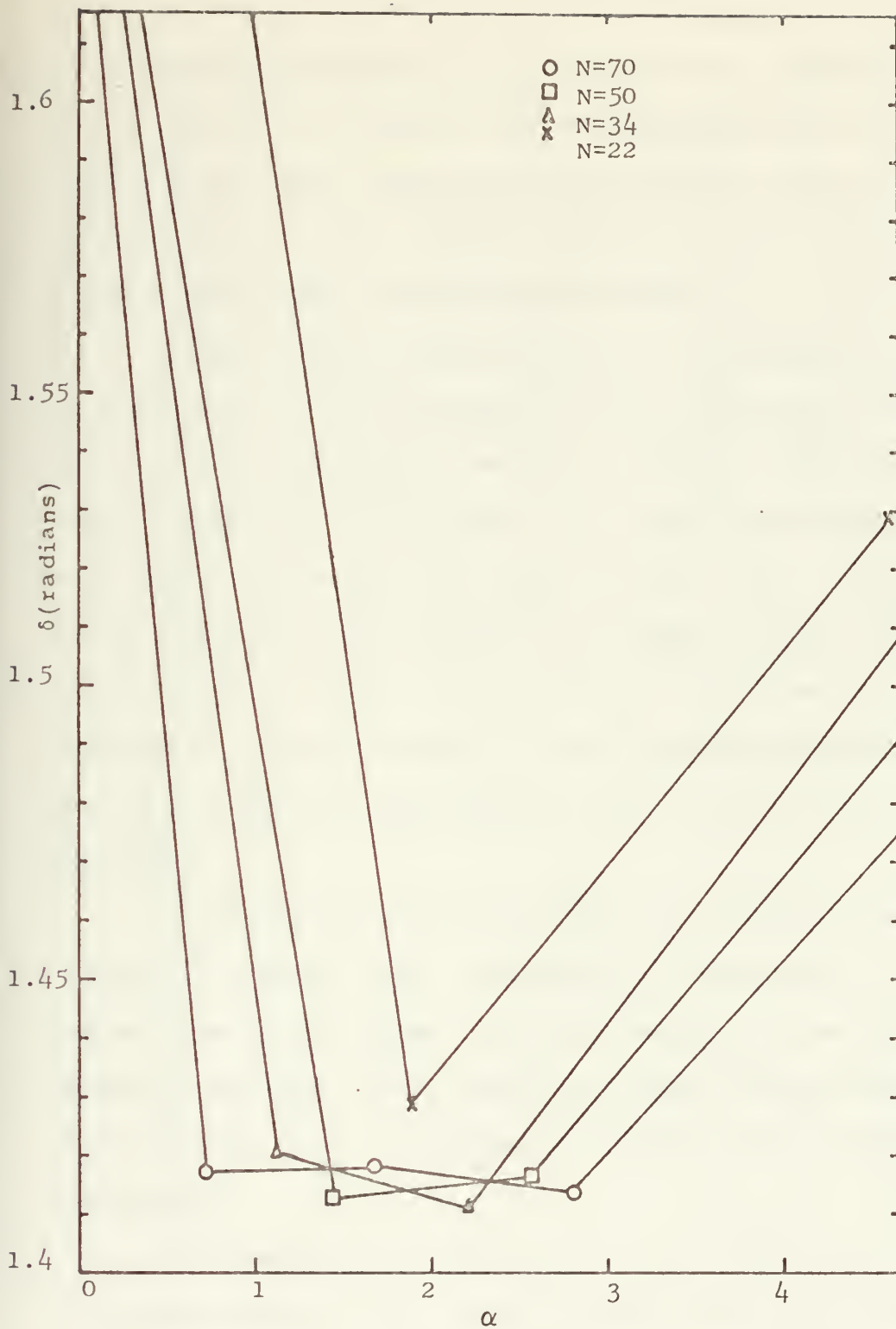


Figure 5. Singlet Phase Shift for e-H as a Function of  $\alpha$   
 $k = 0.4$ .



Although they do not discuss it, close examination of the results of the Harris calculation of e-H singlet phase shifts by Oberoi and Callaway [13] using the close-coupling approximation seems to indicate that their results may be as much as 4-5% less than Schwartz's at  $k = 0.8$ , although their graphical presentation of results makes such a comparison difficult.

Appeal to experiment to resolve the ambiguity is fruitless at this time for the difference in total scattering cross-section at  $k = 0.8$  for the two values of  $\delta$ , 0.886 and 0.761 is only about 3%, far less than the accuracy of any experiments conducted to date [33]. The experiments report results about 15% less than those of Schwartz and Armstead at the upper energy limit and it is worth noting that the present result is also lower than that of Schwartz's. However because of the large experimental errors reported ( $\geq 20\%$ ) the significance of this fact, if any, cannot be estimated.

Based on the results available it seems more wishful than logical to ascribe more significance to the plateaus in the  $N = 70$  curves than to the minima and in the absence of the results of Schwartz the lower value would most likely have been chosen as the most probable value. Therefore the minima will be chosen for consistency.

The extrema of the curves for phase shift vs.  $\alpha$  generally are minima except at the lowest energies calculated and they seem to trend downward, so in most cases the value of the phase shift for  $N = 70$  can probably be taken as an upper limit except for  $k \leq 0.2$  where it seems to be a lower limit. Where an unambiguous



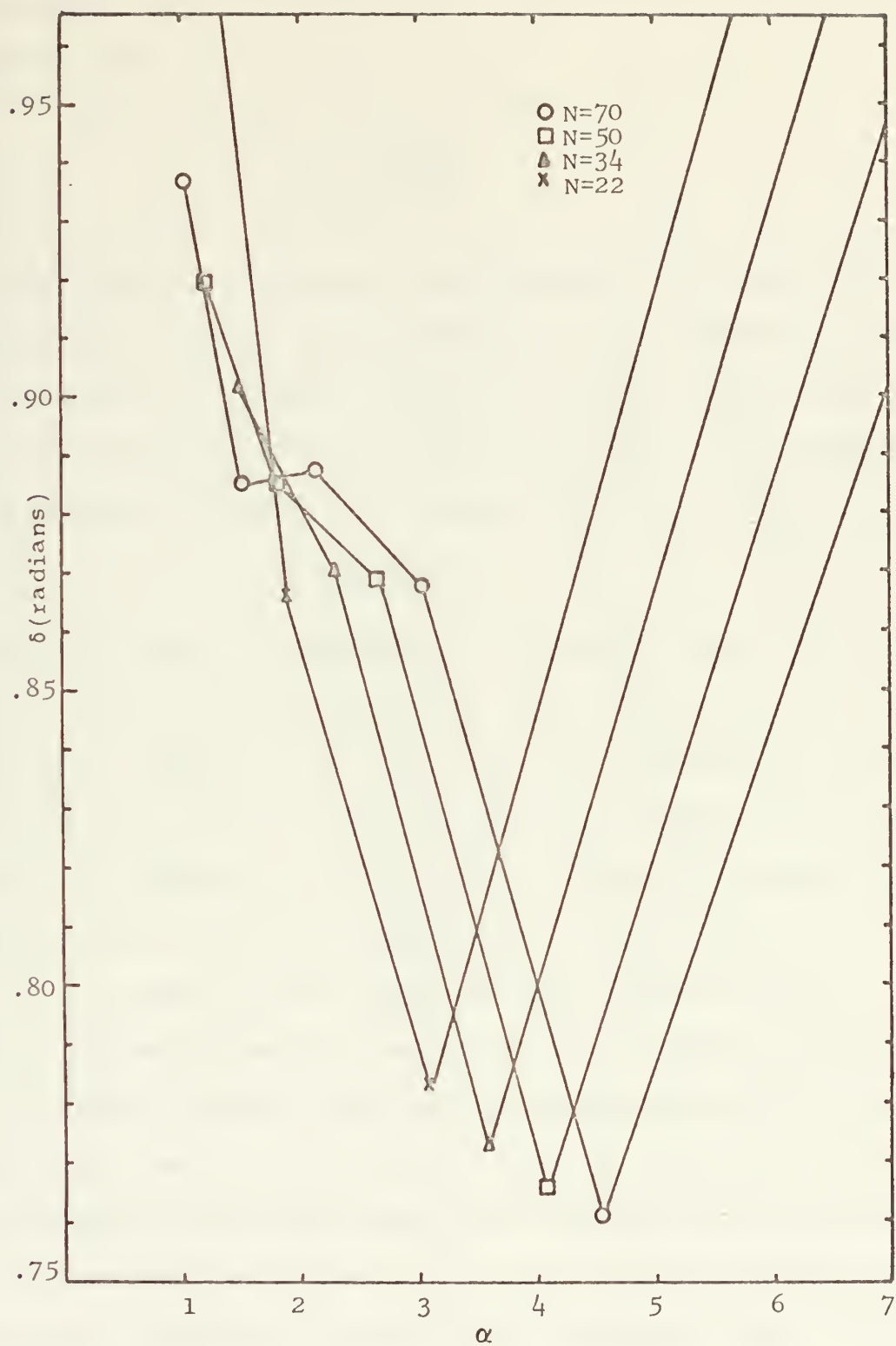


Figure 6. Singlet Phase Shift for e-H as a Function of  $\alpha$   
 $k = 0.8$ .





convergence could be established it seemed to be about as the sequence  $1/N$ .

The scattering length is defined to be

$$a_o = \lim_{k \rightarrow 0} \frac{\tan \delta_o}{k} \quad . \quad (59)$$

In the present calculation it seemed natural to evaluate the scattering length for e-H scattering by simply evaluating  $(\tan \delta)/k$  for a succession of small values of  $k$  and extrapolating the results to  $k = 0$ . This was done for the case  $N = 70$  and the smallest value of  $k$  used was .000412. The extrapolation to  $k = 0$  gave

$$a_o = -6.02181(1)$$

where the figure in parentheses is the uncertainty in the last digit. This value differs by about 1% from the value  $a_o = -5.965$  reported by Schwartz [12]. Note that the uncertainty reported above is the uncertainty arising from the extrapolation to zero and is not necessarily an indication of absolute accuracy. The extrapolation used in evaluating  $a_o$  is shown in Figure 7.

It should be noted that the difficulties with the Harris method discussed above should not be peculiar to this choice of trial wave function, for since the Hamiltonian (30) is the exact Hamiltonian for any two-electron system the eigenvalue calculation should lead to the same effects described above for any choice of trial wave function as long as it meets the usual boundary conditions and is based on a quadratically integrable basis. Perhaps by using some approximate Hamiltonian the eigenvalue situation would be improved but the loss of accuracy from this approximation would probably offset any gains from improved eigenvalue behavior.



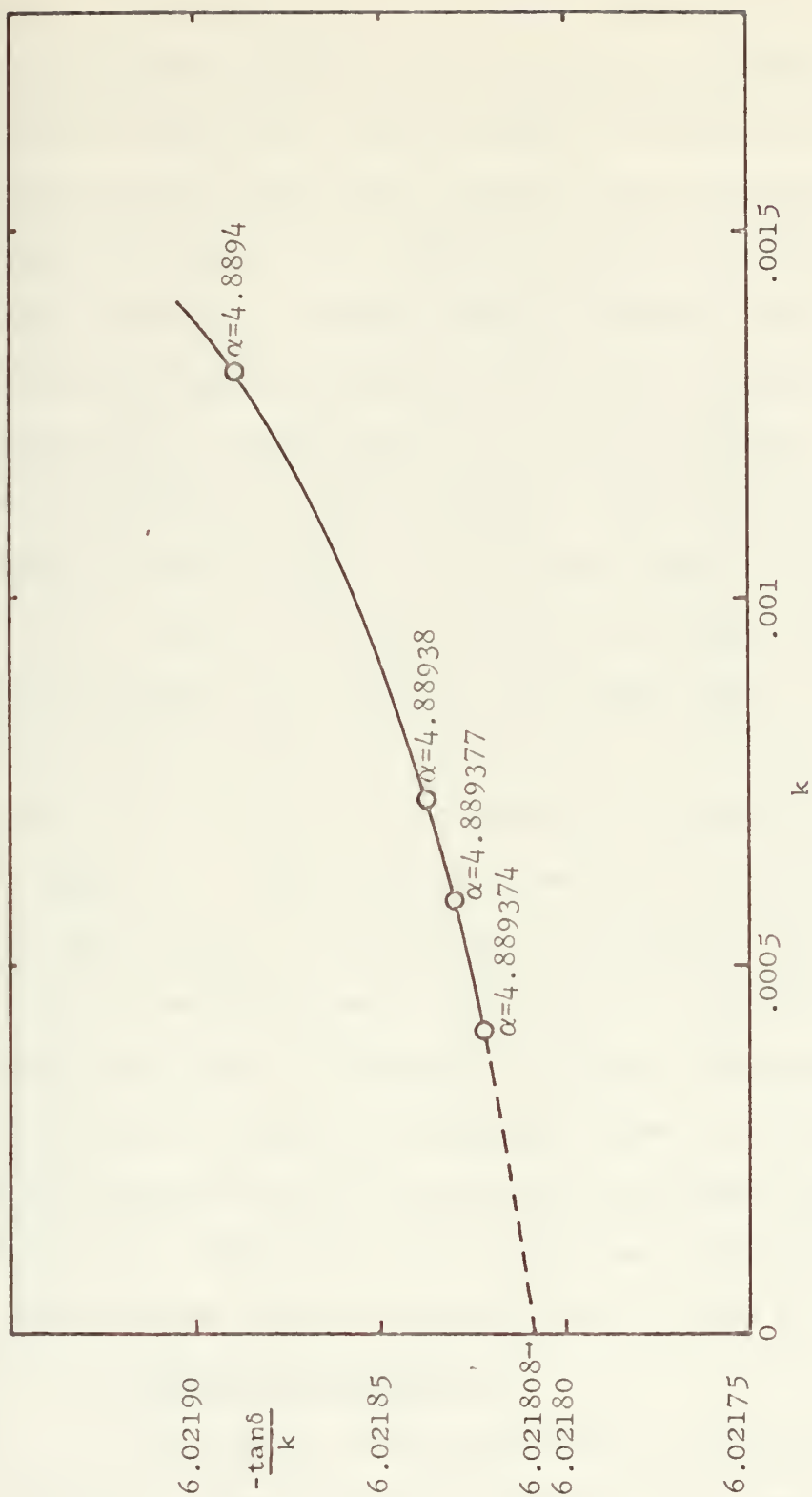


Figure 7. Evaluation of e-H Singlet Scattering Length.  
N=70



The results for the triplet phase shifts are much as has been described above for the singlet case except that the curves seem to trend upward toward maxima for values of  $k$  larger than was found in the singlet case. Since in the triplet case the electron spins are parallel the effective repulsion between the electrons due to the Pauli principle tends to improve the convergence. Thus, while the qualitative picture is similar to that of the singlet scattering, the ambiguities are much less severe. Figure 8 shows the eigenvalue trajectories for  $N = 70$ . Note that there is no trajectory that reaches  $k = 0$ , the lowest one just barely passing  $k = 0.1$ . Hence it was not possible to evaluate the triplet scattering length as was done for the singlet case. Figures 9 and 10 show plots of phase shift vs.  $\alpha$  for  $k = 0.4$  and  $0.8$ . Finally, the curve of  $\delta$  vs.  $k$  for both singlet and triplet scattering is shown in Figure 11. The resonances shown on the plot are discussed in the next section. In each case one resonance which has been reported elsewhere as being just below the excitation threshold was observed in this calculation to be just above and is so indicated on the plot by the vertical dashed lines. It is believed that increasing the basis set size would bring these values below the threshold. The singlet and triplet phase shifts are tabulated and compared with those of Schwartz [12] in Table II.

## 2. Scattering Resonances

The present calculation offers a feature not found in Schwartz's calculation--the localization of real scattering resonances. There is probably no theoretical reason why the Kohn method should not show the resonances, however since they are very



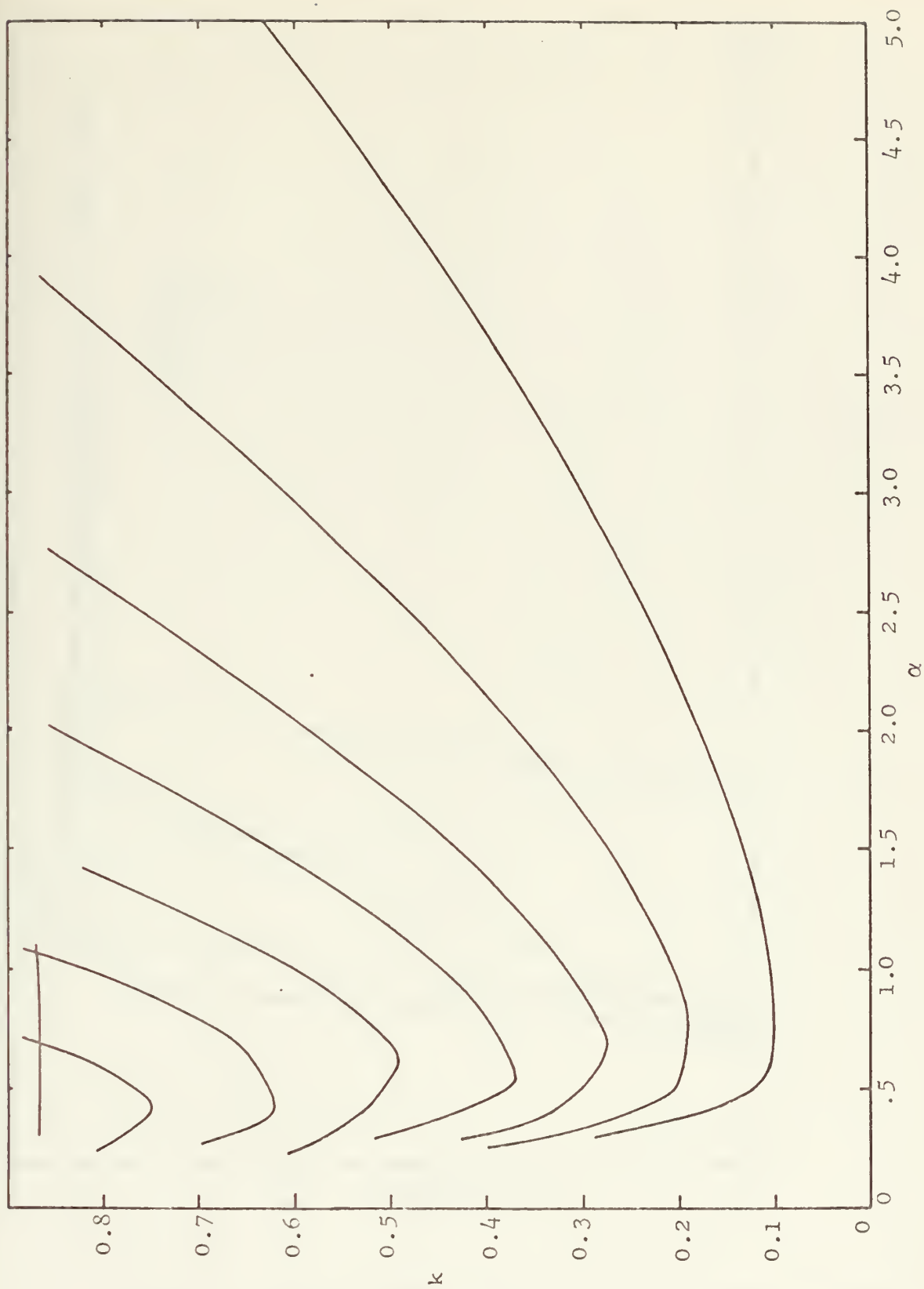


Figure 8. Eigenvalue Trajectories for Triplet e-H System.  $N=70$





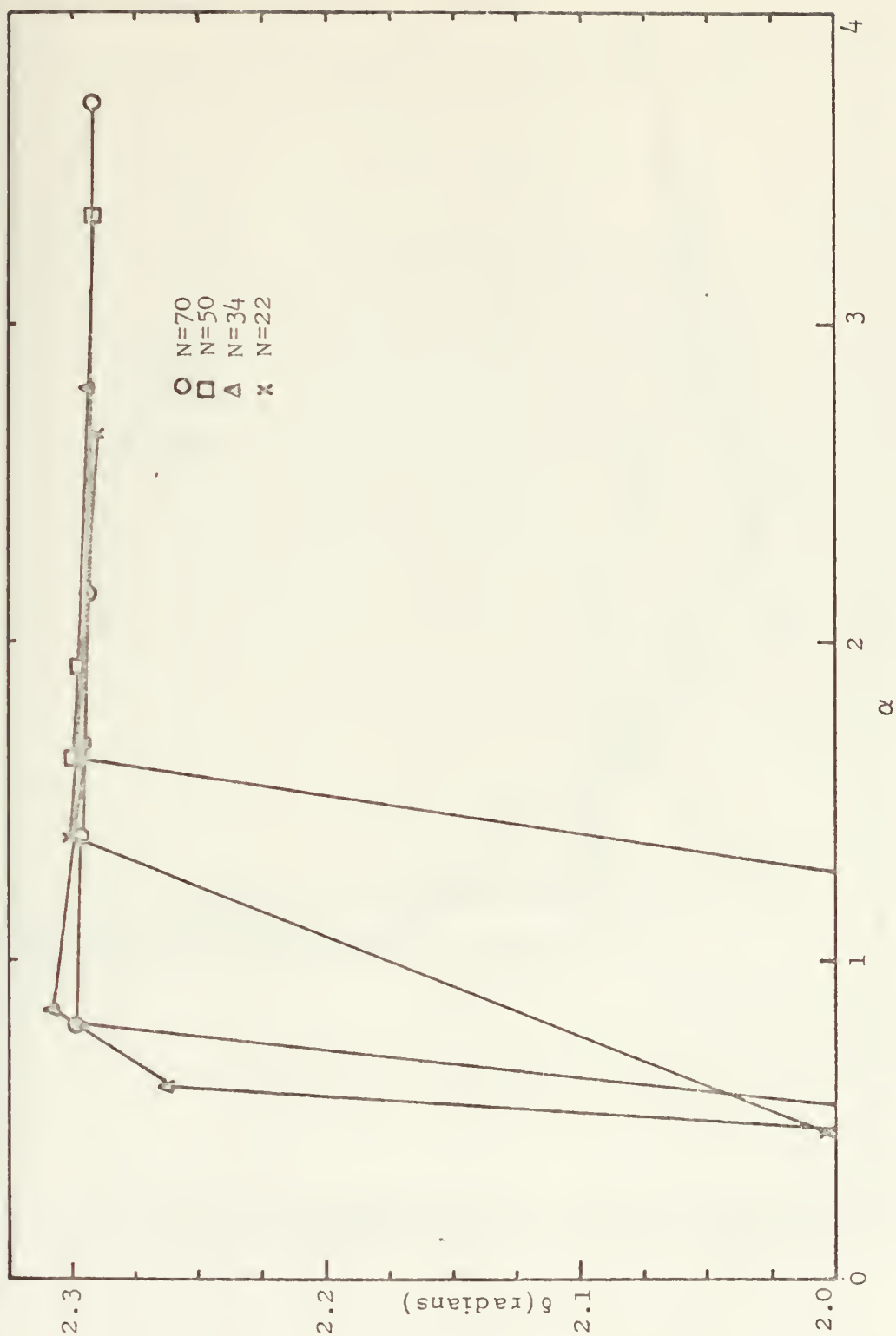


Figure 9. Triplet Phase Shift for e-H as a Function of  $\alpha$ .  
 $k = 0.4$



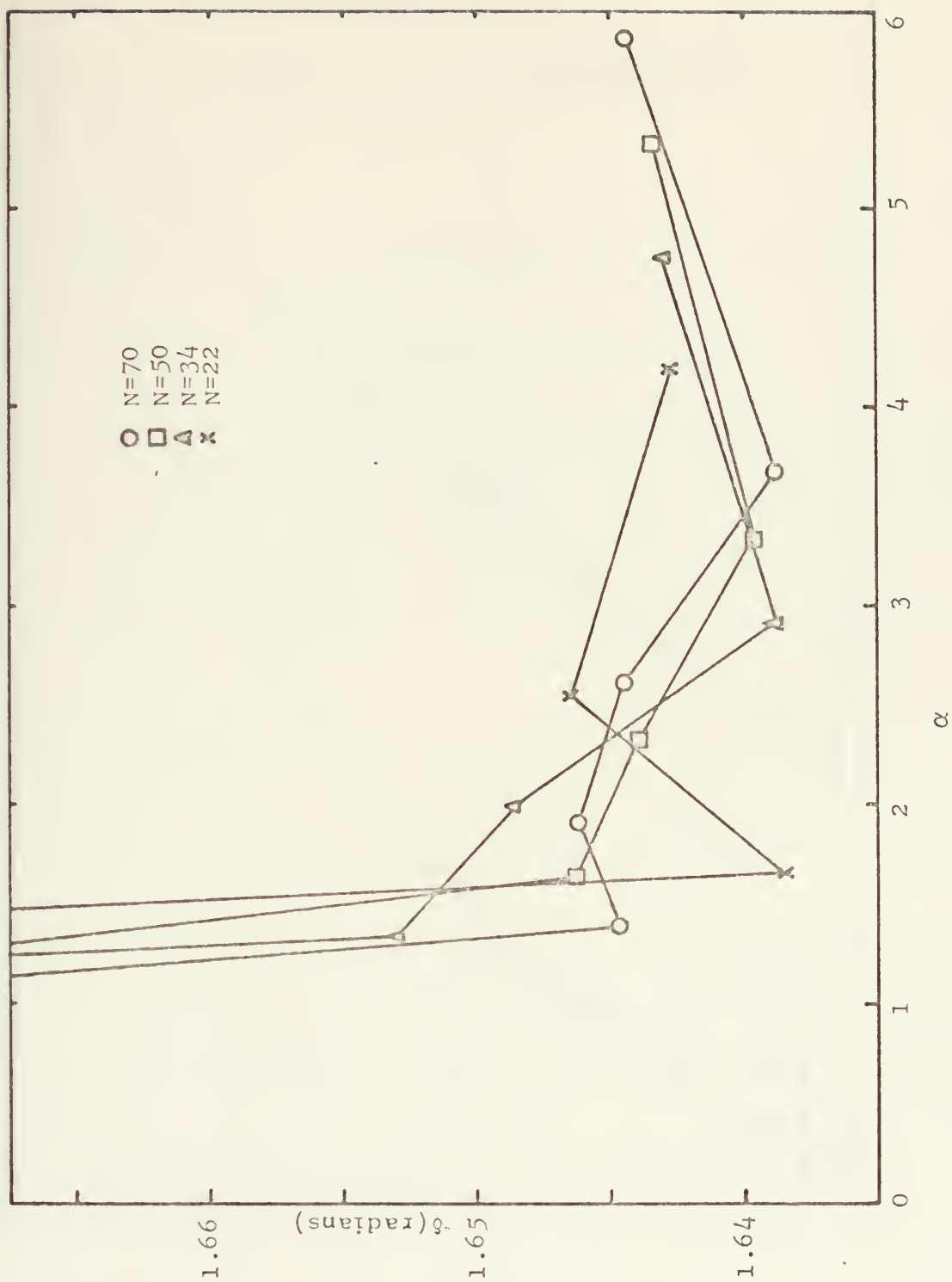


Figure 10. Triplet Phase Shift for e-H as a Function of  $\alpha$ .  
 $k = 0.8$



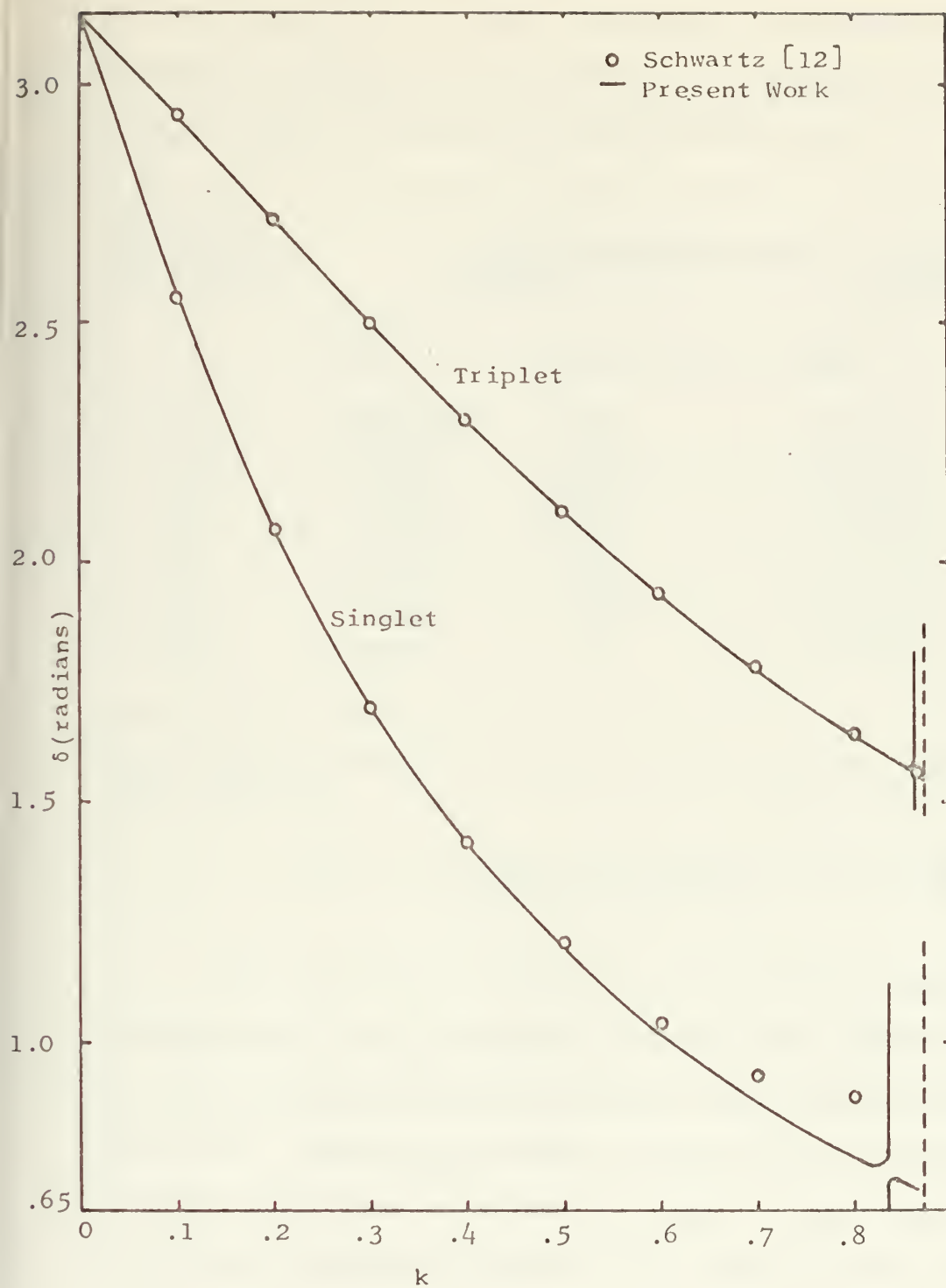


Figure 11. Calculated Phase Shifts for e-H Scattering.



narrow [18,34,35] it is quite likely that they simply were not resolved. It might also be difficult to distinguish them from the spurious ones characteristic of such calculations.

Incident Electron Wave Number	<u>Scattering Phase Shift in Radians</u>			
	Singlet		Triplet	
	Present Work	Schwartz[12]	Present Work	Schwartz[12]
0.1	2.566(5) <sup>a</sup>	2.553	2.9386(5)	2.9388
0.2	2.067(4)	2.0673	2.7187(7)	2.7171
0.3	1.696(6)	1.6964	2.5013(7)	2.4496
0.4	1.414(6)	1.4146	2.2980(5)	2.2938
0.5	1.194(7)	1.202	2.1093(3)	2.1046
0.6	1.020(4)	1.041	1.9321(5)	1.9329
0.7	.878(3)	.930	1.7772(4)	1.7797
0.8	.761(4)	.886	1.6389(5)	1.643
0.9	.693(7)	---	1.5622(6)	1.563

---

<sup>a</sup>The figures in parentheses represent the uncertainty in the last digit reported.

Table II. Singlet and Triplet Phase Shifts for e-H Elastic Scattering.

The existence of scattering resonances has long been associated with the auto-ionizing states of the compound system [36] and recent experiments and calculations have confirmed this [35,37,38]. Auto-ionizing states (in the case of  $H^-$  they are more properly called auto-detaching) are those in which the total energy of the system exceeds the ground state energy by more than the ionization energy of the two-electron system but in which both electrons are in excited states. Such states can decay non-radiatively when one electron's excess energy is transferred to the other which is then ejected from the atom while the first reverts to the one-electron ground state. Such states are normally





extremely short lived, typical lifetimes often being several orders of magnitude less than the normally allowed radiative transitions [39]. Clearly an electron captured momentarily into such a state will be considerably delayed in its passage by the atom, suffering a correspondingly greater phase shift, and thus show a resonant behavior in the cross section. Since these states lie above the one electron ionization potential and are extremely short-lived they are often referred to as quasi-bound [40].

Figures 3 and 8 show the evidence of such states in the singlet and triplet structure of  $H^-$ . They are the broad shallowly curved trajectories lying just below the excitation threshold in each case.

Since these states do lie above the ionization potential of  $H^-$  and thus among a continuum of states, one expects from the Hylleraas-Undheim theorem [32] that such states would not be well approximated by an eigenvalue trajectory until after all lower lying states had been. The reasons for this not being so are not well understood, however Holþien and Midtal [40] have found that if the trial wave functions include an appropriate mix of the one electron state functions (i.e.,  $1sns$ ,  $n > 1$ , and also  $1s1s$ ,  $2s2s$ ,  $2p2p$ , etc.) that the eigenvalues corresponding to the autoionizing states begin stabilizing long before those of many lower lying states. They conjecture that this probably occurs because the equal treatment of the two electrons leads to an approximate orthogonalization to the lower states. The limits approached by these trajectories may not be upper bounds however.



That such conditions occur in the present problem is most likely a result of the use of Hylleraas-type trial functions, which can be combined to approximate the one-electron orbitals needed to satisfy the condition set by Holþien and Midtal above.

In the present calculation two resonances were resolved within the e-H elastic scattering range. One in the singlet states was observed at  $k = 0.83713$  which corresponds to a bound state energy of  $E = -.149610$  atomic units ( $1 \text{ a.u.} = 27.2 \text{ eV}$ ). A second in the triplet states was observed at  $k = 0.86418$  which corresponds to  $E = -.126596 \text{ a.u.}$  In addition there were two such states identified just above the excitation threshold which probably correspond to levels predicted just below the threshold by others [38]. In all likelihood a larger basis than those used here would give a better approach to the results reported by others. Since the means of locating these resonances was from a bound state calculation no estimate of their width can be given. A characteristic of these calculations is that the phase shifts associated with a particular eigenvalue trajectory tend to be rather independent. Thus evaluating a phase shift at a value of  $k$  corresponding to a resonance energy but at a value of  $\alpha$  corresponding to a normal (i.e., non-resonant) eigenvalue trajectory appears to show little or no evidence of the resonance. Although the non-resonant and resonant trajectories sometimes do cross, no conscious attempt to evaluate the phase shift at such a crossing point was made since in the eigenvalue method used (Jacobi variable threshold [41] the eigenvectors found for degenerate or nearly degenerate eigenvalues may be grossly inaccurate (Ref. 41, p. 281) and thus the phase shift calculated at



this point would be difficult to interpret. The independence of the phase shifts corresponding to different trajectories is probably related to the orthogonality properties inherent in the eigenvalue problem and discussed above but beyond this it is not well understood. Table III summarizes the results for the e-H resonances and compares them with other calculations and with such experimental data as is available.

### 3. H<sup>-</sup> Energy Levels

As shown in Appendix C and as demonstrated in the last section, the first part of the Harris prescription involves what amounts to a variational calculation of the bound state energies. Reports of such calculations abound in the literature, commencing with Hylleraas [20] and continuing to the present, and have attained a high degree of accuracy. Hence the results obtained here are of no more than passing interest except that they arise as a natural by-product of the Harris method, and this fact seems not to have been mentioned previously in the literature concerning the Harris method. Considering that no special pains were taken to assure accuracy (other than the normal and reasonable ones discussed in Appendix D) the energy results are surprisingly accurate, and since they are obtained with no additional effort from the phase shift calculation it seems worthwhile to discuss them briefly here.

Pekeris [46] has reported a calculation of the ground state energies of He and H<sup>-</sup> in which he used matrices of up to order 1078 and was at great pains to achieve the maximum possible accuracy. He reports the ground state of H<sup>-</sup> from this calculation to be



Energy of Auto-ionizing State (a.u.)<sup>b</sup>

Resonance Level	Incident Electron Wave Number <sup>a</sup>	Present Work	Bhatia [42]	O'Malley [43]	Burke [44]	Hol6ien [40]	Experiment (McGowan [45])
Singlet							
1	0.8373	-149610	-14878	-14872	-14866	-14883	-149
2	0.8725	-1194	-12601	-12596	-12595		
Triplet							
1	0.86418	-126596	-127108	-127005	-12699		
2	0.8725	-1194	-125092	-125065			

<sup>a</sup> Given as calculated in the present work. The second level in each case is clearly too high since the first excitation level of H is at  $k = 0.86603$ .

<sup>b</sup> Below the ionization energy of H.

Table III.  $H^-$  Auto-ionizing Levels Corresponding to e-H Scattering Resonances





$-.52775097$  a.u. In the present work a value of  $-.5277477$  a.u. was obtained with an order 70 matrix.

As an example of the bound state results obtainable, Figures 12 and 13 show the negative energy structure for the singlet ( $N = 70$ ) and triplet ( $N = 50$ ) calculations. Not all the detail is included in the region near zero energy because the large number of eigenvalues in that region makes it very difficult to sort out the eigenvalue trajectories. Note that the lower eigenvalues clearly exhibit the broad minima alluded to in section 1. This characteristic of the trajectories is even more pronounced in the case of helium, which will now be discussed.

## B. ELECTRON-HELIUM ION SCATTERING

### 1. Phase Shifts

In principle the only difference between scattering electrons from helium ions and from hydrogen is the presence of the long range Coulomb force in the former. This effect is accounted for in the form chosen for the asymptotic part of the trial wave function and once the more difficult problem of numerically evaluating the resultant integrals is solved, one expects the procedure to be straightforward and to yield results whose accuracy is degraded only by the relative inaccuracy of numerical integration vs. exact integration. Appendix D contains extensive discussion of the method of evaluating the numerical integrals and assuring their accuracy, and it appears that a high degree of confidence can be placed in them. Nevertheless the results of these phase shift calculations are not so accurate as the hydrogen ones, if one accepts the results of Burke and Taylor [18] as the most accurate



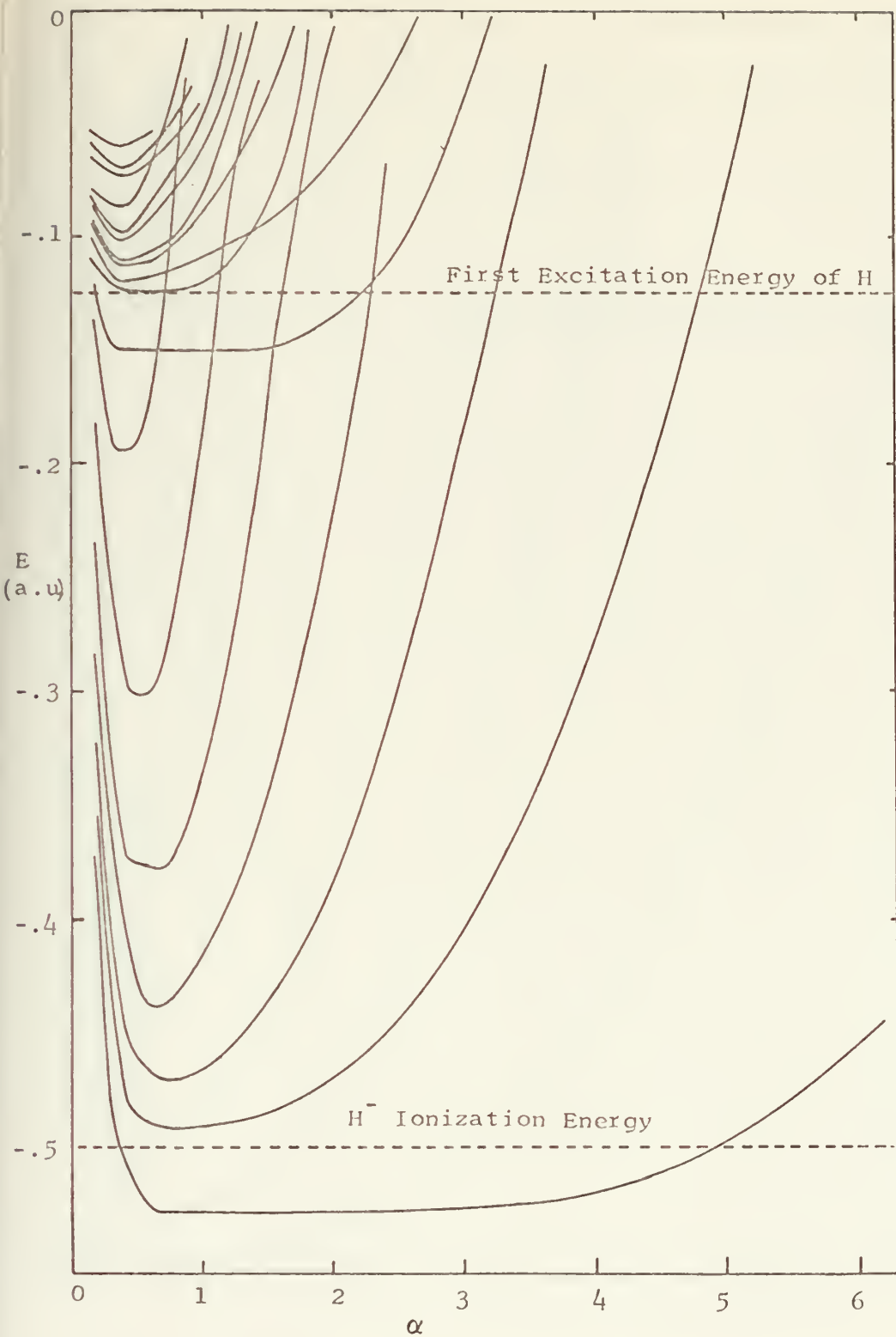


Figure 12. Singlet Energy Levels for  $H^-$ .  $N = 70$



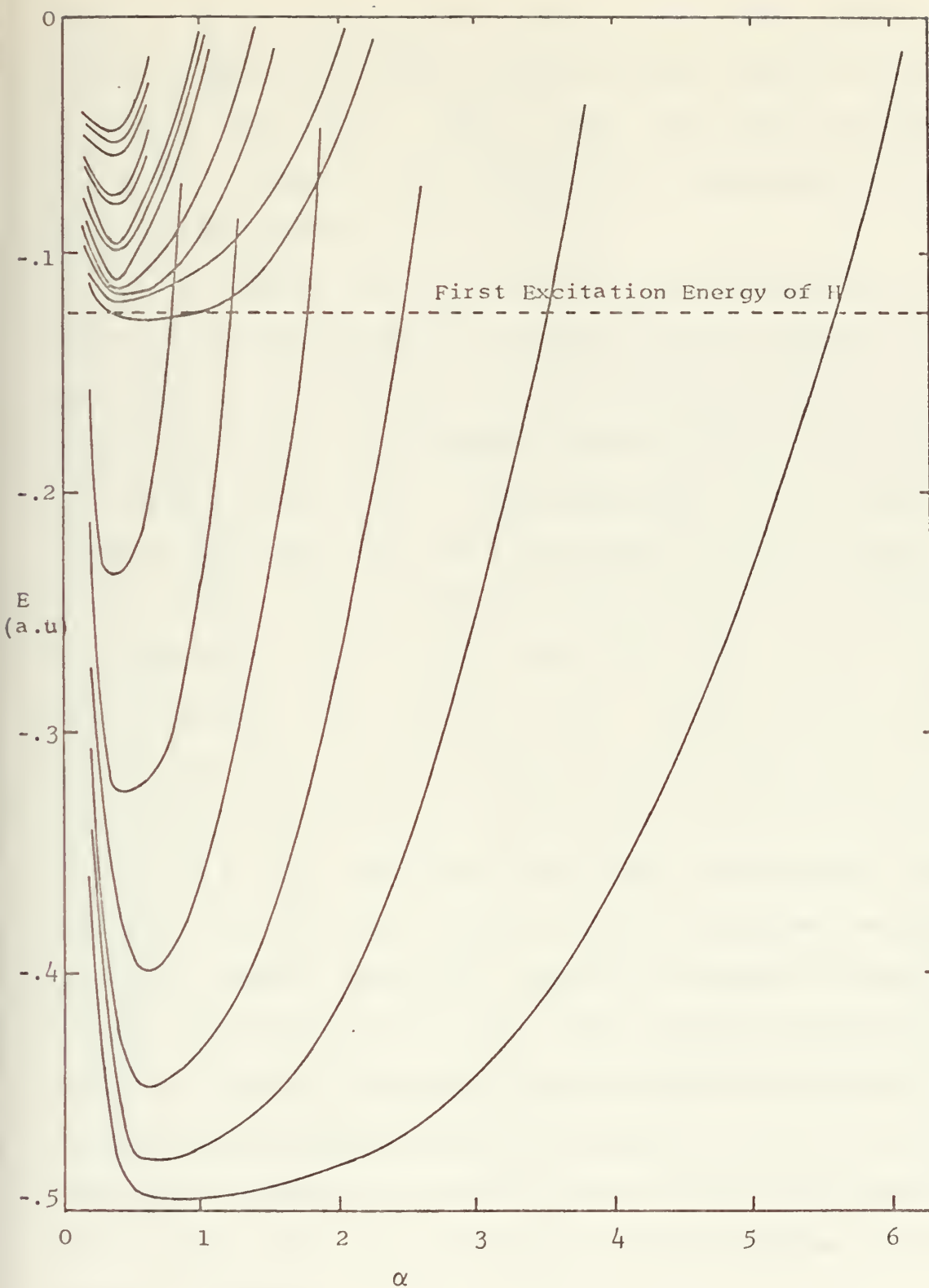


Figure 13. Triplet Energy Levels for  $H^-$ .  $N = 50$



to date. The close agreement of their results with those of others by different methods [35,44] indicates that this confidence is probably well placed. Thus it would appear that the Coulomb force has an effect on the accuracy of the calculation beyond what is initially expected.

As Figures 14 and 17 show, the eigenvalue trajectory situation is somewhat improved in the case of helium, owing to the existence of a complete set of two electron bound states in the region below the first ionization potential of He. Nevertheless the singlet phase shifts at low energy appear to be as much as an order of magnitude larger than the results reported by Burke and Taylor. Because the calculation gives only  $\tan\delta$  the value of  $\delta$  is uncertain by  $\pm n\pi$ , and the choice of  $\delta$  to be .4 at  $k = 0.2$  is in closer agreement with Burke and Taylor. However the slope of the  $\delta$  vs.  $k$  curve at  $k = 0.2$  was measured and its value seems to support the higher value chosen. At higher energy the convergence appears to be to a result about 5-10% higher than that reported by Burke and Taylor, although the existence of the scattering resonances at higher energies undoubtedly affects the results and makes comparison difficult in this region. The existence of the resonances makes more likely the possibility of attempting to evaluate the phase shift at a nearly degenerate eigenvalue, with its concomitant inaccurate eigenvector which may further confuse the picture. Typical plots of  $\delta$  vs.  $\alpha$  for singlet  $e\text{-He}^+$  scattering are shown in Figures 15 and 16.

A similar but (not unexpectedly) less severe situation exists with the triplet scattering. Figures 18 and 19 show typical triplet plots of  $\delta$  vs.  $\alpha$ .





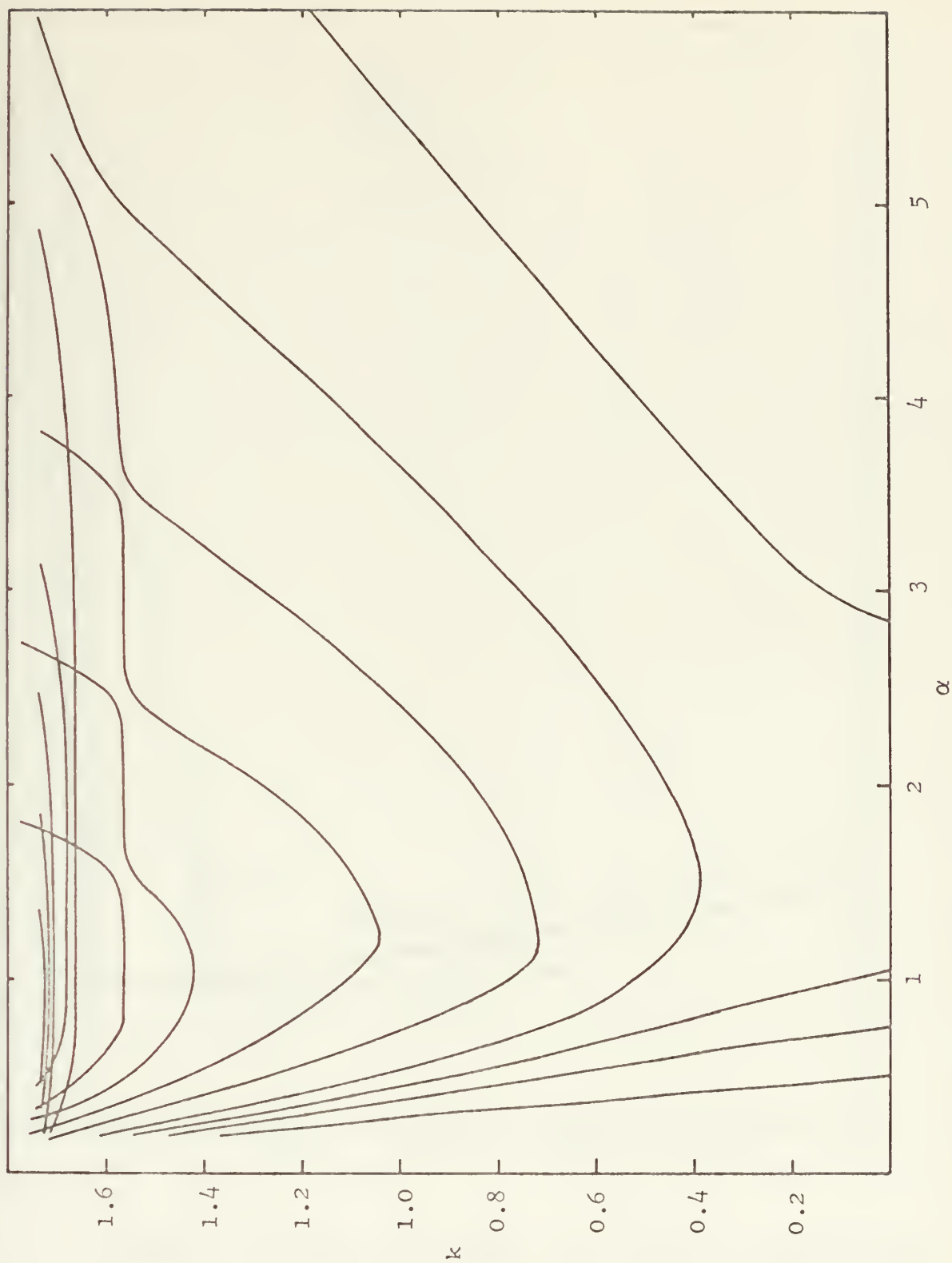


Figure 14. Eigenvalue Trajectories for Singlet  $e\text{-He}^+$  System.  $N=70$





Figure 15. Singlet Phase Shift for  $e\text{-He}^+$  as a Function of  $\alpha$ .  
 $k = 0.8$



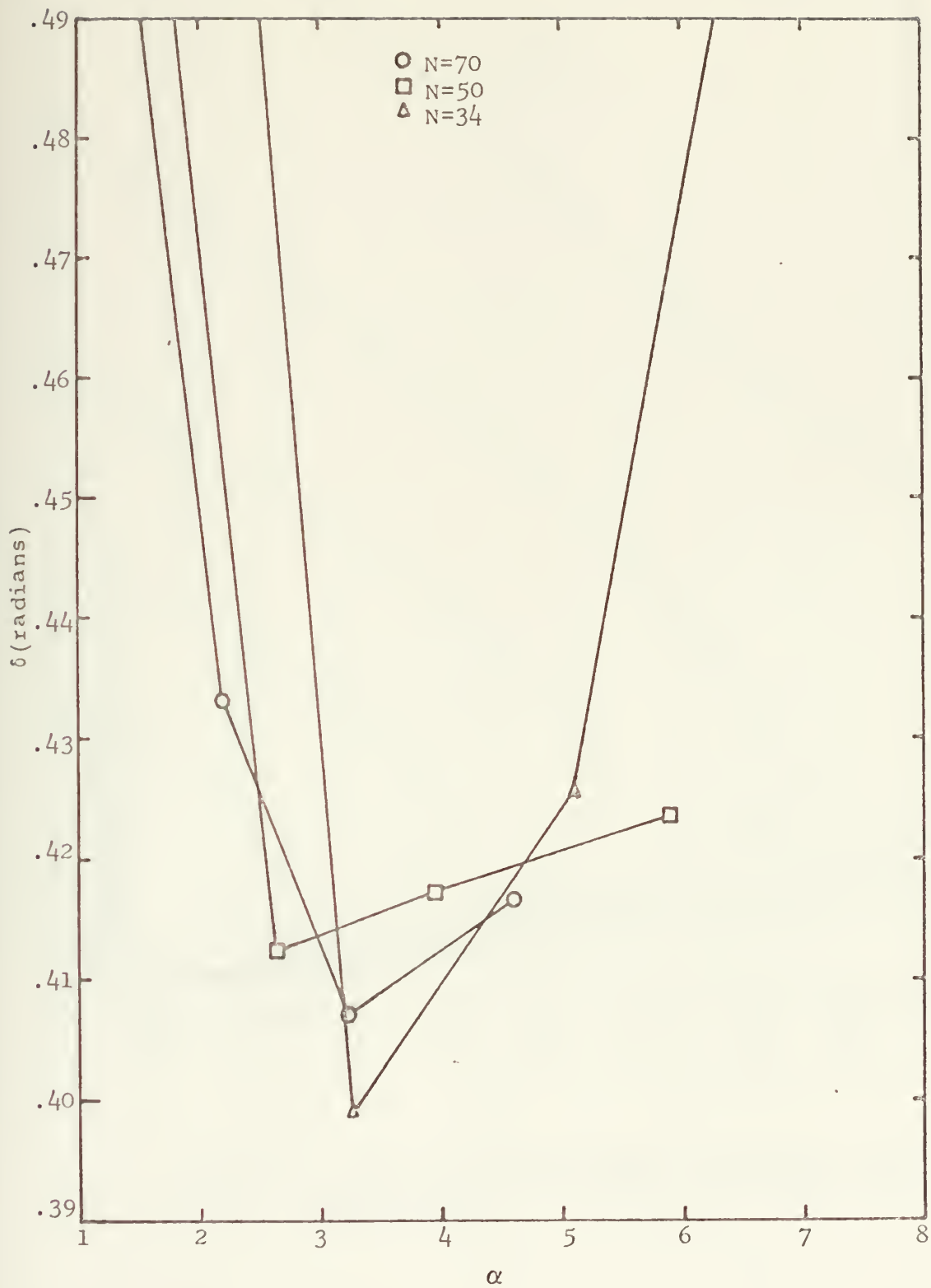


Figure 16. Singlet Phase Shift for  $e\text{-He}^+$  as a Function of  $\alpha$ .  
 $k = 1.4$



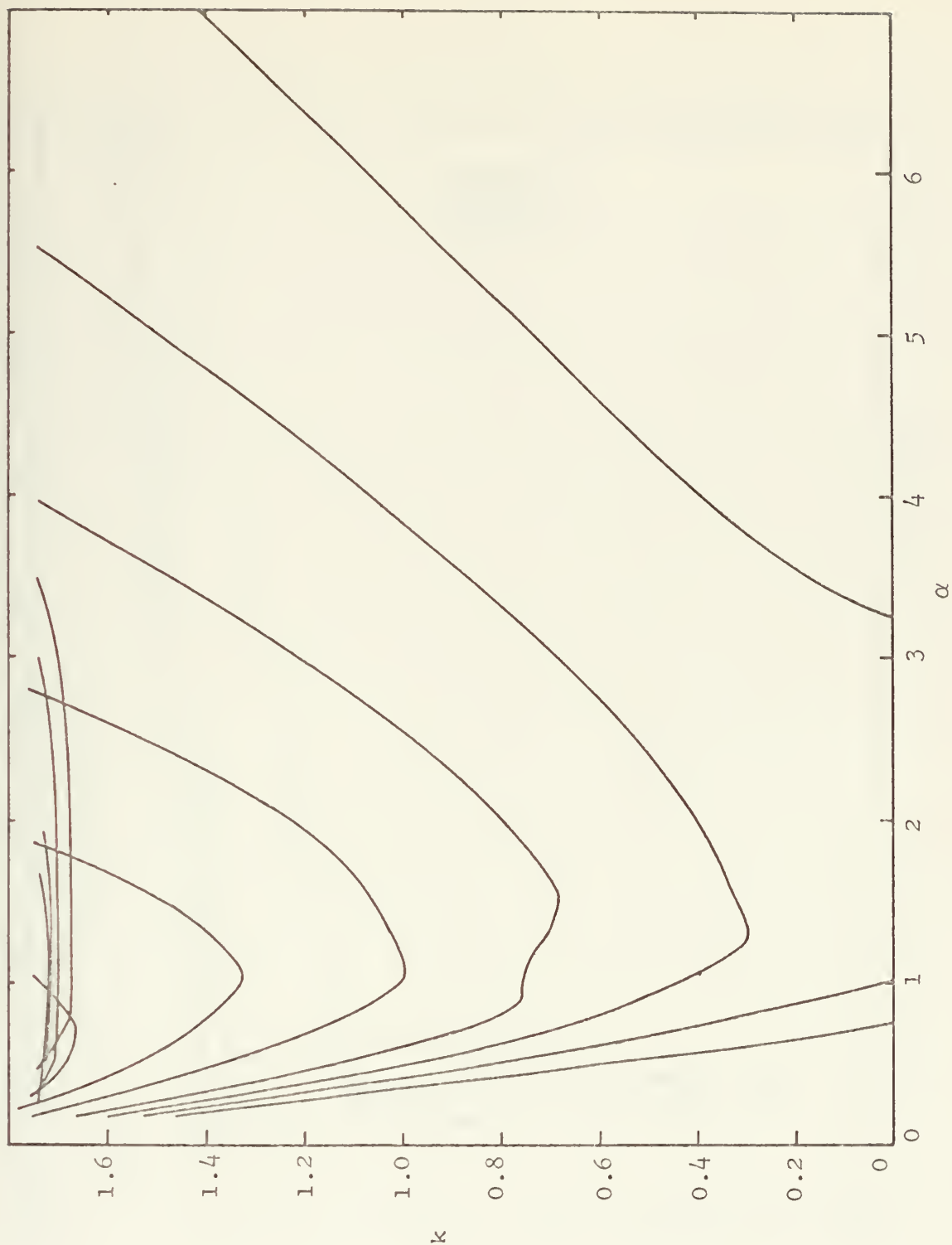


Figure 17. Eigenvalue Trajectories for Triplet  $e\text{-He}^+$  System.  $N=50$





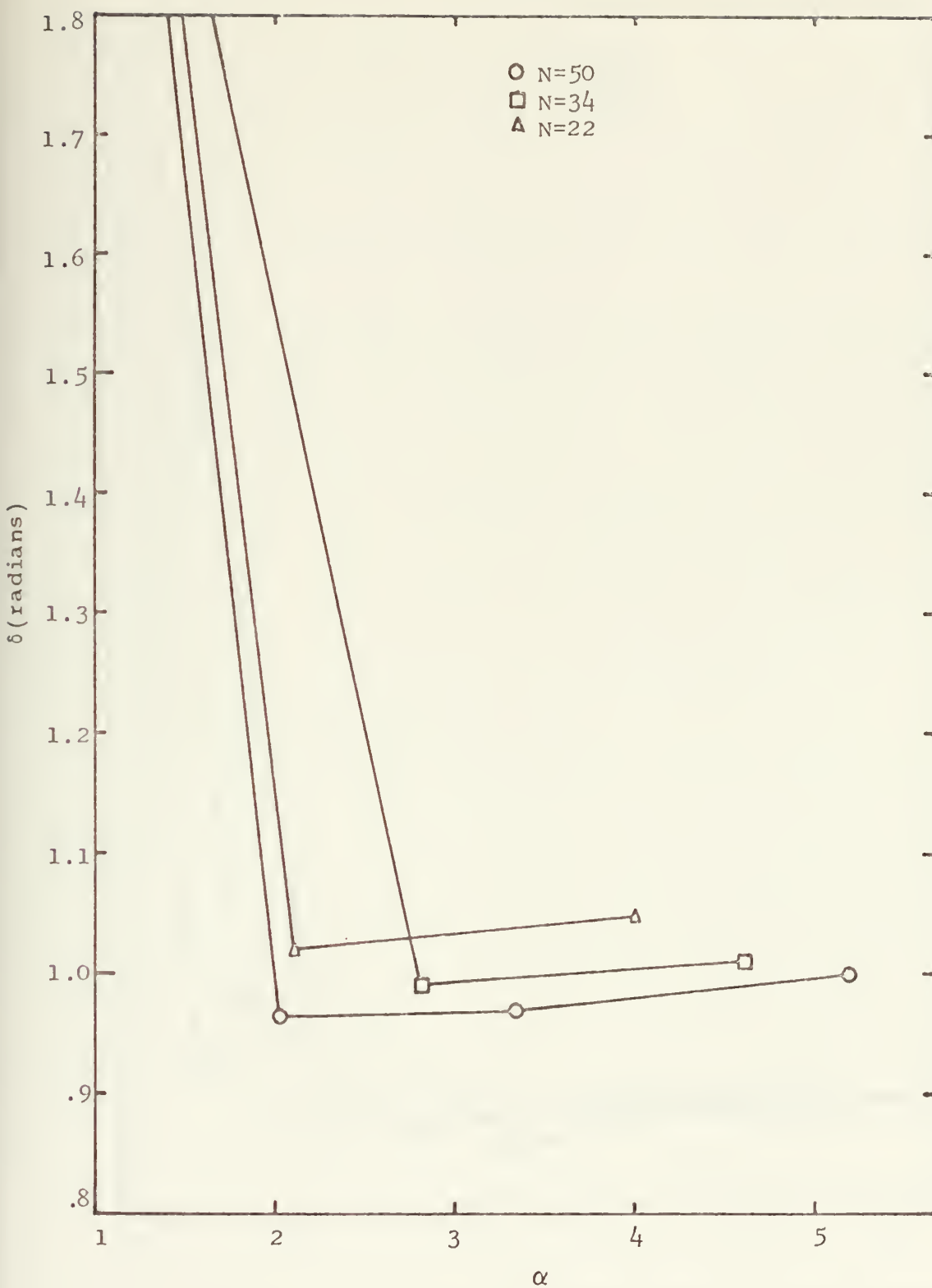


Figure 18. Triplet Phase Shift for  $e\text{-He}^+$  as a Function of  $\alpha$ .  
 $k = 0.8$



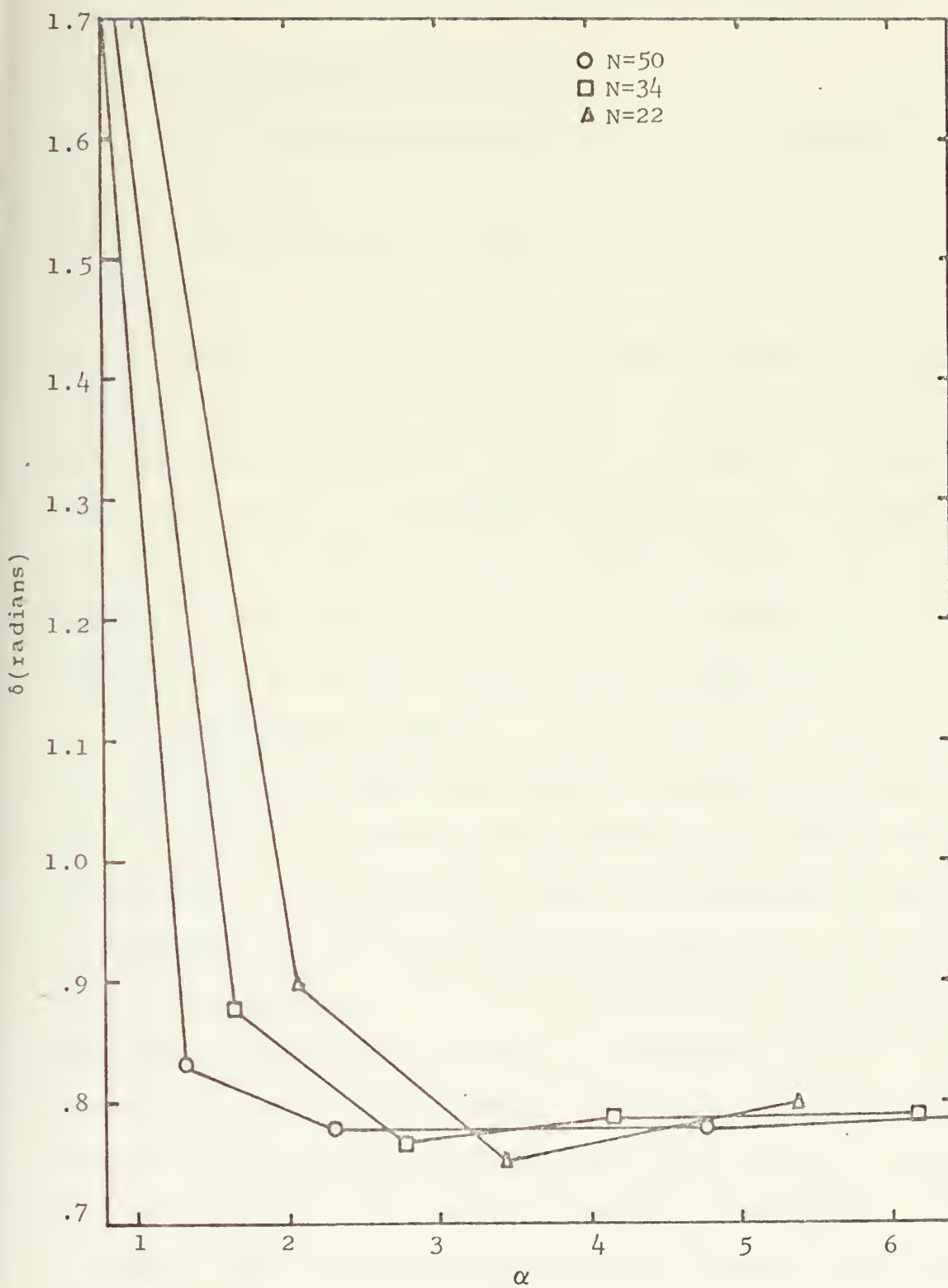


Figure 19. Triplet Phase Shift for  $e\text{-He}^+$  as a Function of  $\alpha$ .  
 $k = 1.4$



Results of the present calculation are presented and compared with those of Burke and Taylor in Table IV and plotted in Figure 20.

## 2. Scattering Resonances

It was possible to identify six singlet resonances and four triplet resonances. As shown in Table V the agreement with the results of Burke and McVicar [44] and others [37,40,42,43,47] is quite good.

Burke and McVicar give the energies of seven and five resonances for singlet and triplet states, respectively. As in the hydrogen case an additional resonance level could be identified just above the excitation threshold by examining the energy level plots for each system. Again as in the hydrogen, these levels would probably appear just below the excitation threshold if the calculation were done with a sufficiently large basis set.

## 3. Helium Energy Levels

The helium energy spectrum has been even more extensively calculated than has hydrogen [20,46,48,49]. The most accurate such calculation is that of Pekeris [46] who has reported a value of -2.903724375 a.u. for the ground state energy of He. After applying mass polarization and relativistic corrections and correcting for the Lamb shift, he finds a value of  $1.98310687 \times 10^5 \text{ cm}^{-1}$  for the ground state of He, which compares with the experimental determination by Herzberg [50] of  $1.983108 \times 10^5 \pm .05 \text{ cm}^{-1}$ . Similarly, for the  $2^3\text{S}$  state of He, Pekeris obtained -2.17522937822 a.u. or  $3.84566 \times 10^4 \text{ cm}^{-1}$  while Herzberg measured  $3.845473 \times 10^4 \pm .05 \text{ cm}^{-1}$ . In the present calculation -2.90372410 a.u. and -2.175191 a.u. were



# Scattering Phase Shift in Radians

Incident Electron Wave Number	Singlet		Triplet	
	Present Work	Burke and Taylor [18]	Present Work	Burke and Taylor [18]
0.2	3.5(9) <sup>a</sup>		4.1(9)	
0.4	.98(4)		1.469(8)	
0.4472		.4217		.9088
0.6	.63(2)		1.108(6)	
0.6325		.4092		.8873
0.7746		.3989		.8649
0.8	.512(8)		.965(6)	
0.8944		.3912		.8462
1.0	.446(7)	.3850	.889(4)	.8253
1.1832		.3780		.7895
1.2	.417(7)		.831(5)	
1.3416		.3779		.7593
1.4	.407(4)		.778(4)	
1.4832		.3910		.7341
1.5811		.2977		
1.6	.348(4)		.730(4)	
1.6553		.3988		
1.6712				.7006
1.6971				.6931
1.7073		.2572		
1.732	.326(3)		.705(4)	

<sup>a</sup>The figures in parentheses represent the uncertainty in the last digit reported.

Table IV. Singlet and Triplet Phase Shifts for e-He<sup>+</sup>  
Elastic Scattering





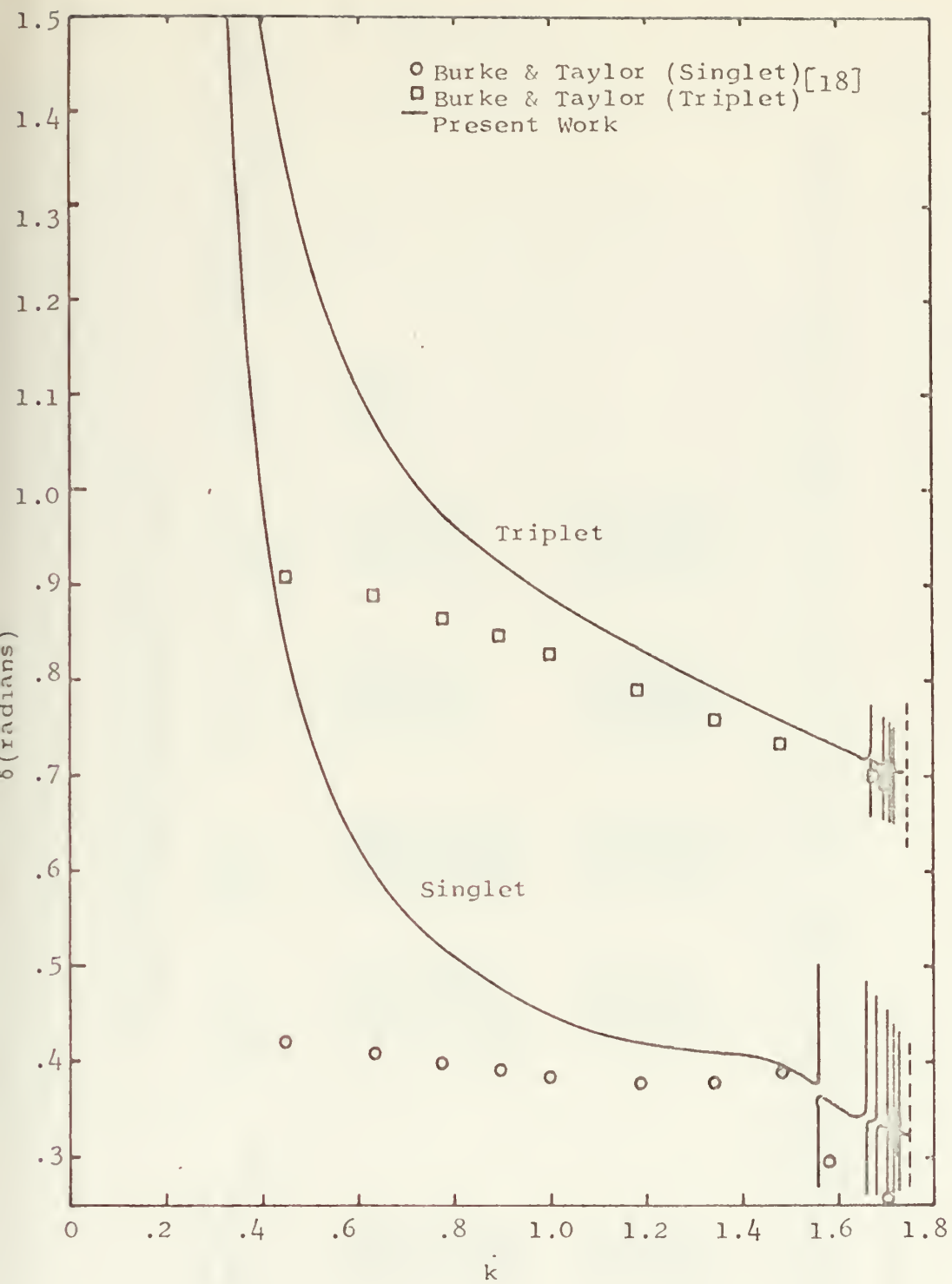


Figure 20. Calculated Phase Shifts for e-He<sup>+</sup> Scattering.



Energy of Auto-ionizing Level (a.u.)<sup>b</sup>

Resonance Level	Incident Electron Wave Number <sup>a</sup>	Present Work	Burke [44]	O'Malley [43]	Bhatia [42]	Holøien [40]	Experiment Simpson [47]	Rudd [37]
Singlet								
1	1.5627	-.7795	-.77637	-.77824	-.77877	-.777	-.775	-.778
2	1.66003	-.62216	-.59461	-.61912	-.62274	-.620		
3	1.67832	-.59162	-.58722	-.58980	-.59003	-.596		-.589
4	1.70439	-.54753	-.54408	-.55006	-.54818			
5	1.71475	-.52982	-.54284	-.54000	-.54487			-.542
6	1.72313	-.51541	-.52580					
7	1.738	-.490	-.52513					-.525
Triplet								
1	1.67179	-.60255	-.60150	-.60240	-.60260			
2	1.69729	-.55960	-.55732	-.56042	-.55976			
3	1.70719	-.54275	-.54797	-.55344	-.54884			
4	1.71729	-.52545	-.53116	-.53092	-.53251			
5	1.744	-.479	-.56437	-.52668	-.52833			

<sup>a</sup> Given as calculated in the present work. The last level in each case is clearly too high since the first excitation level of He<sup>+</sup> is at k = 1.732.

<sup>b</sup> Below the ionization energy of He<sup>+</sup>.

Table V. He Auto-ionizing Levels Corresponding to e-He<sup>+</sup> Scattering Resonances.



obtained for the  $1^1\text{S}$  and  $2^3\text{S}$  levels in He, respectively. Figures 21 and 22 show the calculated energy levels for the singlet and triplet S states of He.



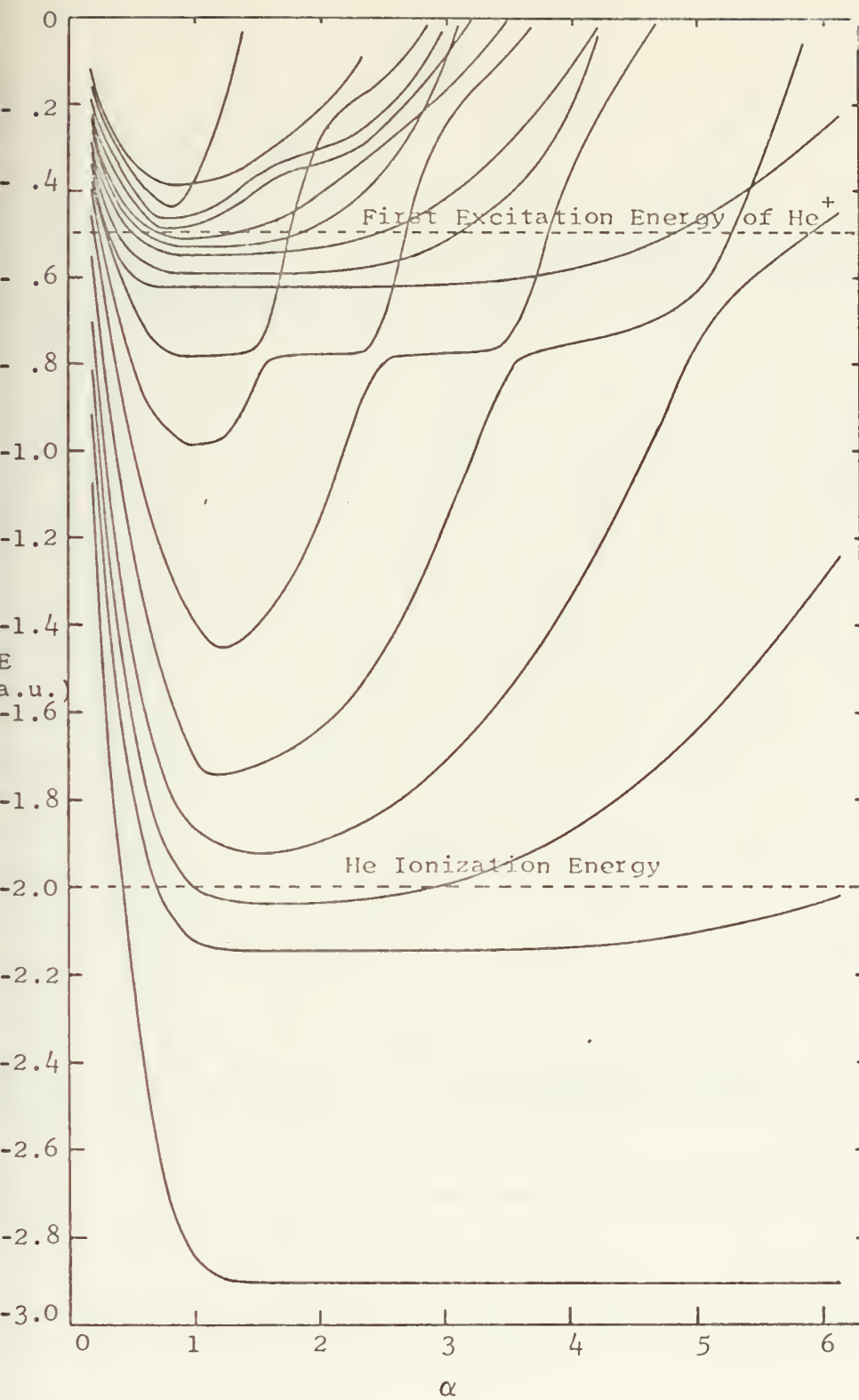


Figure 21. Singlet Energy Levels of He.  $N=70$





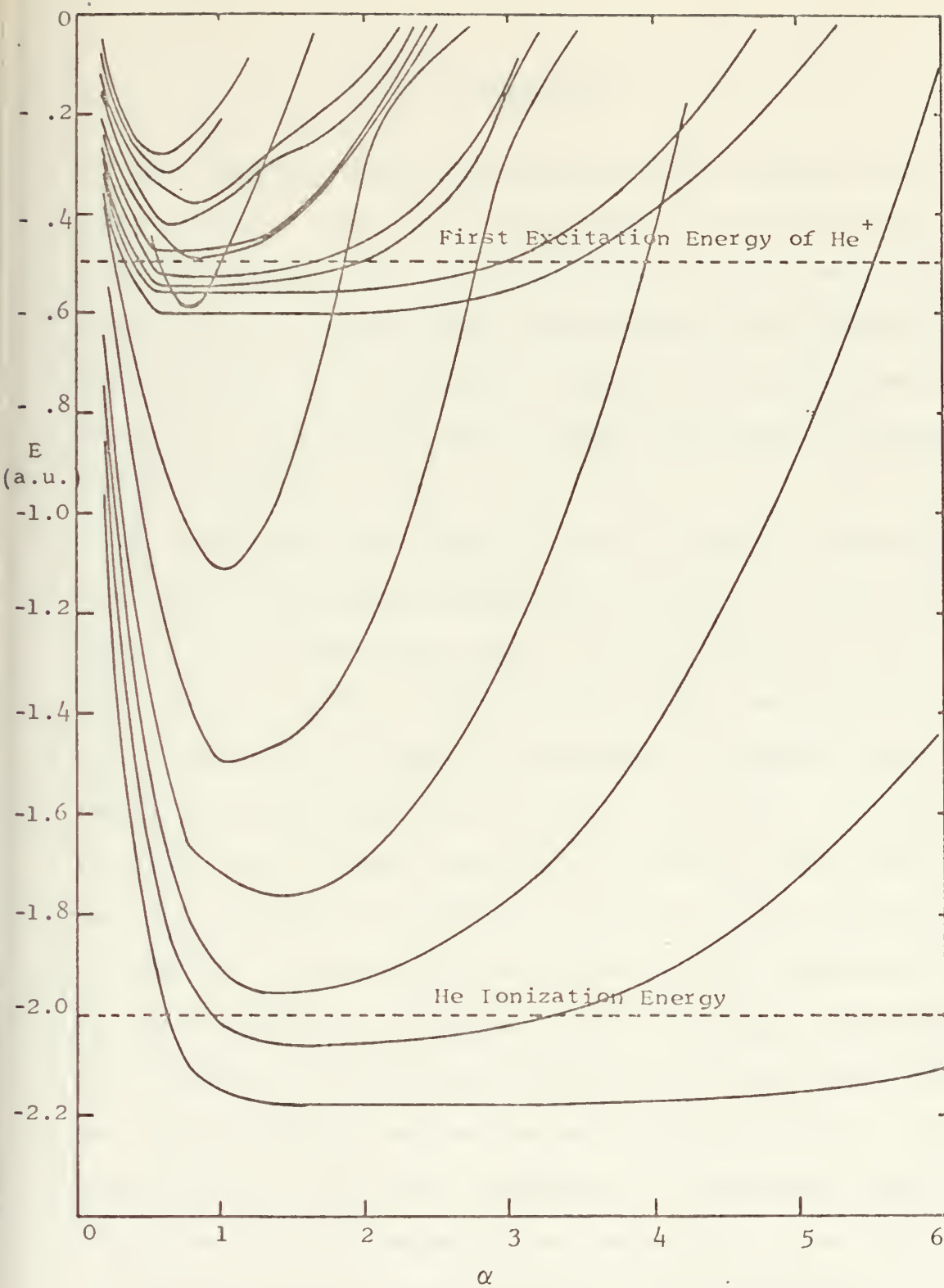


Figure 22. Triplet Energy Levels of He.  $N=50$



#### IV. CONCLUSION

The principle advantage in calculating phase shifts by the Harris method is that it is not required to evaluate matrix elements involving only the asymptotic part of the wave function. This results in a considerable computational simplification but the price paid is that the error is now of first order and hence the method is inherently less accurate than methods dependent on the Kato identity.

An additional disadvantage is that in certain regions there may be a paucity of energy eigenvalues at which to carry out the calculation. Since these eigenvalues are approximations to the compound system energy levels, in those regions where the approximations are good, increasing the number of parameters in the trial wave function may simply make the situation worse. Even in regions rich in eigenvalues the fact that they are related to the bound states may have unpredictable effects on the phase shift calculations.

The Harris method does have a feature that could prove useful in complex systems. Resonances in the scattering cross-section can be uniquely identified as arising from certain bound states of the compound system, such as the auto-ionizing states in the present instance. Since the scattering at a particular energy can be identified with the compound state energy level, when that level is well defined by the trial wave function the correlation with the behavior of the phase shifts in that region will be clear.



Whether the anomalous results for the  $e\text{-He}^+$  system found here are an indication of a defect in the Harris method or due to a subtle error in computation or analysis on the part of the author is not absolutely clear. Although the latter cannot be ruled out, the success of the method in calculating the  $e\text{-H}$  scattering using the same computer program and even, as pointed out in Appendix D, the same integration scheme (on a test basis), seems strong evidence in favor of the former conclusions. A third possibility, of course, is that the results obtained here are correct and the results of Burke and Taylor and others are incorrect. In the absence of experimental evidence to the contrary, the consistency of the other calculations would seem to make this conclusion also unlikely.

Thus it is the tentative conclusion of this thesis, that the Harris method should be applied to electron-ion scattering with some degree of caution.



## APPENDIX A

### Formulae for the Various Matrix Elements

#### 1. $H_{ij}$ and $S_{ij}$

The matrix elements  $\langle \chi_i | H | \chi_j \rangle$  is made up of 52 terms, each of which includes an integral of the form

$$A(\nu, \lambda, \mu) = \int d\vec{r}_1 d\vec{r}_2 e^{-\alpha(r_1+r_2)} r_1^{\nu-2} r_2^{\lambda-2} r_{12}^{\mu-2} \quad (A-1)$$

or

$$B(\nu, \lambda, \mu) = \int d\vec{r}_1 d\vec{r}_2 e^{-\alpha(r_1+r_2)} r_1^{\nu-2} r_2^{\lambda-2} r_{12}^{\mu-2} \cos\theta_{12} . \quad (A-2)$$

The trial wave function is

$$\chi = e^{-\frac{\alpha}{2}(r_1+r_2)} \left( r_1^n r_2^\ell \pm r_1^\ell r_2^n \right) r_{12}^m \quad (A-3)$$

and can be characterized by the three exponents  $n, \ell, m$ . Let  $\chi_i$  be characterized by  $n_i, \ell_i, m_i$  and  $\chi_j$  by  $n_j, \ell_j, m_j$ . With this notation  $H_{ij}$  can be written

$$\begin{aligned} H_{ij} = & - (\alpha^2/4) \cdot A(n_i + n_j + 2, \ell_i + \ell_j + 2, m_i + m_j + 2) \\ & + [\frac{1}{2}\alpha(n_j + 1) - Z] \cdot A(n_i + n_j + 1, \ell_i + \ell_j + 2, m_i + m_j + 2) \\ & + [\frac{1}{2}\alpha(\ell_j + 1) - Z] \cdot A(n_i + n_j + 2, \ell_i + \ell_j + 1, m_i + m_j + 2) \\ & + \frac{1}{2}\alpha m_j \cdot A(n_i + n_j + 2, \ell_i + \ell_j + 3, m_i + m_j) \\ & + \frac{1}{2}\alpha m_j \cdot A(n_i + n_j + 3, \ell_i + \ell_j + 2, m_i + m_j) \\ & - m_j(m_j + \ell_j + n_j + 1) \cdot A(n_i + n_j + 2, \ell_i + \ell_j + 2, m_i + m_j) \\ & - \frac{1}{2}n_j(n_j + 1) \cdot A(n_i + n_j, \ell_i + \ell_j + 2, m_i + m_j + 2) \end{aligned}$$





$$\begin{aligned}
& - \frac{1}{2} l_j (l_j + 1) \cdot A(n_i + n_j + 2, l_i + l_j, m_i + m_j + 2) \\
& + A(n_i + n_j + 2, l_i + l_j + 2, m_i + m_j + 1) \\
& - \frac{1}{2} \alpha m_j \cdot B(n_i + n_j + 2, l_i + l_j + 3, m_i + m_j) \\
& - \frac{1}{2} \alpha m_j \cdot B(n_i + n_j + 3, l_i + l_j + 2, m_i + m_j) \\
& + m_j n_j \cdot B(n_i + n_j + 1, l_i + l_j + 3, m_i + m_j) \\
& + m_j l_j \cdot B(n_i + n_j + 3, l_i + l_j + 1, m_i + m_j) \\
& - \frac{1}{4} \alpha^2 \cdot A(l_i + l_j + 2, n_i + n_j + 2, m_i + m_j + 2) \\
& + [\frac{1}{2} \alpha (l_j + 1) - Z] \cdot A(l_i + l_j + 1, n_i + n_j + 2, m_i + m_j + 2) \\
& + [\frac{1}{2} \alpha (n_j + 1) - Z] \cdot A(l_i + l_j + 2, n_i + n_j + 1, m_i + m_j + 2) \\
& + \frac{1}{2} \alpha m_j \cdot A(l_i + l_j + 2, n_i + n_j + 3, m_i + m_j) \\
& + \frac{1}{2} \alpha m_j \cdot A(l_i + l_j + 3, n_i + n_j + 2, m_i + m_j) \\
& - m_j (m_j + l_j + n_j + 1) \cdot A(l_i + l_j + 2, n_i + n_j + 2, m_i + m_j) \\
& - \frac{1}{2} l_j (l_j + 1) \cdot A(l_i + l_j, n_i + n_j + 2, m_i + m_j + 2) \\
& - \frac{1}{2} n_j (n_j + 1) \cdot A(l_i + l_j + 2, n_i + n_j, m_i + m_j + 2) \\
& + A(l_i + l_j + 2, n_i + n_j + 2, m_i + m_j + 1) \\
& - \frac{1}{2} \alpha m_j \cdot B(l_i + l_j + 2, n_i + n_j + 3, m_i + m_j) \\
& - \frac{1}{2} \alpha m_j \cdot B(l_i + l_j + 3, n_i + n_j + 2, m_i + m_j) \\
& + m_j l_j \cdot B(l_i + l_j + 1, n_i + n_j + 3, m_i + m_j) \\
& + m_j n_j \cdot B(l_i + l_j + 3, n_i + n_j + 1, m_i + m_j) \\
& \pm \{ \frac{1}{4} \alpha^2 \cdot A(n_i + l_j + 2, l_i + n_j + 2, m_i + m_j + 2) \\
& + [\frac{1}{2} \alpha (l_j + 1) - Z] \cdot A(n_i + l_j + 1, l_i + n_j + 2, m_i + m_j + 2) \\
& + [\frac{1}{2} \alpha (n_j + 1) - Z] \cdot A(n_i + l_j + 2, l_i + n_j + 1, m_i + m_j + 2)
\end{aligned}$$



$$\begin{aligned}
& + \frac{1}{2} \alpha m_j \cdot A(n_i + \ell_j + 2, \ell_i + n_j + 3, m_i + m_j) \\
& + \frac{1}{2} \alpha m_j \cdot A(n_i + \ell_j + 3, \ell_i + n_j + 2, m_i + m_j) \\
& - m_j(m_j + n_j + \ell_j + 1) \cdot A(n_i + \ell_j + 2, \ell_i + n_j + 2, m_i + m_j) \\
& - \frac{1}{2} \ell_j(\ell_j + 1) \cdot A(n_i + \ell_j, \ell_i + n_j + 2, m_i + m_j + 2) \\
& - \frac{1}{2} n_j(n_j + 1) \cdot A(n_i + \ell_j + 2, \ell_i + n_j, m_i + m_j + 2) \\
& + A(n_i + \ell_j + 2, \ell_i + n_j + 2, m_i + m_j + 1) \\
& - \frac{1}{2} \alpha m_j \cdot B(n_i + \ell_j + 2, \ell_i + n_j + 3, m_i + m_j) \\
& - \frac{1}{2} \alpha m_j \cdot B(n_i + \ell_j + 3, \ell_i + n_j + 2, m_i + m_j) \\
& + m_j \ell_j \cdot B(n_i + \ell_j + 1, \ell_i + n_j + 3, m_i + m_j) \\
& + m_j n_j \cdot B(n_i + \ell_j + 3, \ell_i + n_j + 1, m_i + m_j) \\
& - \frac{1}{4} \alpha^2 \cdot A(\ell_i + n_j + 2, n_i + \ell_j + 2, m_i + m_j + 2) \\
& + [\frac{1}{2} \alpha(n_j + 1) - Z] \cdot A(\ell_i + n_j + 1, n_i + \ell_j + 2, m_i + m_j + 2) \\
& + [\frac{1}{2} \alpha(\ell_j + 1) - Z] \cdot A(\ell_i + n_j + 2, n_i + \ell_j + 1, m_i + m_j + 2) \\
& + \frac{1}{2} \alpha m_j \cdot A(\ell_i + n_j + 2, n_i + \ell_j + 3, m_i + m_j) \\
& + \frac{1}{2} \alpha m_j \cdot A(\ell_i + n_j + 3, n_i + \ell_j + 2, m_i + m_j) \\
& - m_j(m_j + n_j + \ell_j + 1) \cdot A(\ell_i + n_j + 2, n_i + \ell_j + 2, m_i + m_j) \\
& - \frac{1}{2} n_j(n_j + 1) \cdot A(\ell_i + n_j, n_i + \ell_j + 2, m_i + m_j + 2) \\
& - \frac{1}{2} \ell_j(\ell_j + 1) \cdot A(\ell_i + n_j + 2, n_i + \ell_j, m_i + m_j + 2) \\
& + A(\ell_i + n_j + 2, n_i + \ell_j + 2, m_i + m_j + 1) \\
& - \frac{1}{2} \alpha m_j \cdot B(\ell_i + n_j + 2, n_i + \ell_j + 3, m_i + m_j) \\
& - \frac{1}{2} \alpha m_j \cdot B(\ell_i + n_j + 3, n_i + \ell_j + 2, m_i + m_j) \\
& + m_j n_j \cdot B(\ell_i + n_j + 1, n_i + \ell_j + 3, m_i + m_j) \\
& + m_j \ell_j \cdot B(\ell_i + n_j + 3, n_i + \ell_j + 1, m_i + m_j) \} \quad (A-4)
\end{aligned}$$



and

$$\begin{aligned}
 S_{ij} = & A(n_i + n_j + 2, \ell_i + \ell_j + 2, m_i + m_j + 2) \\
 & + A(\ell_i + \ell_j + 2, n_i + n_j + 2, m_i + m_j + 2) \\
 & + \{ A(n_i + \ell_j + 2, \ell_i + n_j + 2, m_i + m_j + 2) \\
 & + A(\ell_i + n_j + 2, n_i + \ell_j + 2, m_i + m_j + 2) \} \quad (A-5)
 \end{aligned}$$

Note that if the expression ( 54 ) is used to evaluate the A's and B's that each of the terms in (A-4) and (A-5) above must be divided by  $\alpha^{v+\lambda+\mu}$ .

## 2. $\langle S | (H - E) | \chi \rangle$ and $\langle C | (H - E) | \chi \rangle$

Each of these matrix elements is made up of 26 terms which in turn are made up of an integral of the form (53 a-d) where A's and B's are as defined in ( 44 ) to ( 47 ) and immediately following.

Now letting  $\chi$  in (A-3) above be characterized by  $n, \ell, m$ ,  $\langle S, C | (H-E) | \chi \rangle$  is

$$\begin{aligned}
 \langle S, C | (H-E) | \chi \rangle = & - (\frac{1}{2}\alpha^2 + E) \cdot A_{S,C}(\ell + 1, n + 2, m + 2) \\
 & + [\frac{1}{2}\alpha(\ell + 1) - Z] \cdot A_{S,C}(\ell, n + 2, m + 2) \\
 & + [\frac{1}{2}\alpha(n + 1) - Z] \cdot A_{S,C}(\ell + 1, n + 1, m + 2) \\
 & + \frac{1}{2}\alpha m \cdot A_{S,C}(\ell + 1, n + 3, m) \\
 & + \frac{1}{2}\alpha m \cdot A_{S,C}(\ell + 2, n + 2, m) \\
 & - m(m + \ell + n + 1) \cdot A_{S,C}(\ell + 1, n + 2, m) \\
 & - \frac{1}{2}\ell(\ell + 1) \cdot A_{S,C}(\ell - 1, n + 2, m + 2) \\
 & - \frac{1}{2}n(n + 1) \cdot A_{S,C}(\ell + 1, n, m + 2) \\
 & + A_{S,C}(\ell + 1, n + 2, m + 1)
 \end{aligned}$$



$$\begin{aligned}
& - \frac{1}{2}\alpha m \cdot B_{S,C}(\ell+1, n+3, m) \\
& - \frac{1}{2}\alpha m \cdot B_{S,C}(\ell+2, n+2, m) \\
& + \ell m \cdot B_{S,C}(\ell, n+3, m) \\
& + mn \cdot B_{S,C}(\ell+2, n+1, m) \\
& + \left\{ -\left(\frac{1}{4}\alpha^2 + E\right) \cdot A_{S,C}(n+1, \ell+2, m+2) \right. \\
& + \left[\frac{1}{2}\alpha(n+1) - Z\right] \cdot A_{S,C}(n, \ell+2, m+2) \\
& + \left[\frac{1}{2}\alpha(\ell+1) - Z\right] \cdot A_{S,C}(n+1, \ell+1, m+2) \\
& + \frac{1}{2}\alpha m \cdot A_{S,C}(n+1, \ell+3, m) \\
& + \frac{1}{2}\alpha m \cdot A_{S,C}(n+2, \ell+2, m) \\
& - m(m+\ell+n+1) \cdot A_{S,C}(n+1, \ell+2, m) \\
& - \frac{1}{2}n(n+1) \cdot A_{S,C}(n-1, \ell+2, m+2) \\
& - \frac{1}{2}\ell(\ell+1) \cdot A_{S,C}(n+1, \ell, m+2) \\
& + A_{S,C}(n+1, \ell+2, m+1) \\
& - \frac{1}{2}\alpha m \cdot B_{S,C}(n+1, \ell+3, m) \\
& - \frac{1}{2}\alpha m \cdot B_{S,C}(n+2, \ell+2, m) \\
& + mn \cdot B_{S,C}(n, \ell+3, m) \\
& + \left. ml \cdot B_{S,C}(n+2, \ell+1, m) \right\} \quad (A-6)
\end{aligned}$$

where it is assumed  $A_S, B_S$  are chosen when the left hand side is  $\langle S | (H-E) | \chi \rangle$  and  $A_C, B_C$  when it is  $\langle C | (H-E) | \chi \rangle$ .

### 3. Determination of the Required Integrals

Clearly not every term in the above matrix elements requires a different integral. Many of them are identical or have zero





coefficient. For example, for the  $3^4$  element basis set ( $M = 5$ ), while there are 595 independent elements each in  $\underline{H}$  and  $\underline{S}$ , representing 52 terms and 4 terms each, respectively, or a total of more than 33,000 terms, only about 700, or slightly more than two percent, use different integrals and all 700 different integrals can be generated using the recursion relations proved in Appendix B by actually carrying out the evaluation of about 100 integrals for which  $\mu = 2$ . Similarly, in evaluating  $\langle S | (H-E) | \chi \rangle$  and  $\langle C | (H-E) | \chi \rangle$ , where there are  $3^4$  elements in each expression, each element in turn made up of 26 terms, for a total of 1768 integrals required, only 268, or slightly less than one sixth are distinct and again, using the recursion relations only 103 terms for  $\mu = 2$  need be evaluated explicitly and they can all be found from 36 different numerical integrals. Nevertheless it is the numerical evaluation of these integrals which overwhelmingly dominates the time required to solve the complete problem and hence the requirement only to evaluate those terms needed.

To insure that no terms were missed in computing the integral tables, preliminary computer programs were written to examine each of the matrix elements and to display in tabular form which integrals were needed to construct the matrix elements for a given basis set size. Tabulated were all distinct integrals required for which the coefficient was non-zero in at least one case plus those required in order that the recursion relations could be used to generate the terms required for  $\mu = 2$ . From this information the integral table programs were constructed so that only those terms required were actually calculated, and none that would be required was omitted.



## APPENDIX B

### Integral Recursion Relations

#### 1. Recursion Relations for $\mu > 2$ [51]

Consider the integrals

$$A(\nu, \lambda, \mu) = \int d\vec{r}_1 d\vec{r}_2 r_1^{\nu-2} r_2^{\lambda-2} r_{12}^{\mu-2} F(r_1, r_2) \quad (\text{B-1})$$

and

$$B(\nu, \lambda, \mu) = \int d\vec{r}_1 d\vec{r}_2 r_1^{\nu-2} r_2^{\lambda-2} r_{12}^{\mu-2} F(r_1, r_2) \cos\theta_{12} \quad (\text{B-2})$$

and rewrite (B-1) in the form

$$A(\nu, \lambda, \mu) = \int r_1^{\nu-2} r_2^{\lambda-2} r_{12}^{\mu-4} (r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_{12}) F(r_1, r_2) d\vec{r}_1 d\vec{r}_2$$

using the law of cosines. This transforms immediately to

$$A(\nu, \lambda, \mu) = A(\nu+2, \lambda, \mu-2) + A(\nu, \lambda+2, \mu-2) - 2B(\nu+1, \lambda+1, \mu-2). \quad (\text{B-3})$$

Similarly  $B(\nu, \lambda, \mu)$  becomes

$$B(\nu, \lambda, \mu) = B(\nu+2, \lambda, \mu-2) + B(\nu, \lambda+2, \mu-2) - 2 \int r_1^{\nu-1} r_2^{\lambda-1} r_{12}^{\mu-4} F(r_1, r_2) \cos^2\theta_{12} d\vec{r}_1 d\vec{r}_2.$$

Let the integral in the third term be designated  $I$ , then

$$I = A(\nu+1, \lambda+1, \mu-2) - \int r_1^{\nu-1} r_2^{\lambda-1} r_{12}^{\mu-4} F(r_1, r_2) \sin^2\theta_{12} d\vec{r}_1 d\vec{r}_2.$$

Now recall that the angular part of the  $d\vec{r}_1 d\vec{r}_2$  integration is

simply  $\sin\theta_{12} d\theta_{12}$ , whence the angular part of the second term in  $I$  is

$$\begin{aligned} & \int (r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_{12})^{\frac{\mu-4}{2}} \sin^2\theta_{12} d\theta_{12} \\ &= \frac{1}{\mu-2} \frac{1}{r_1 r_2} \int \left[ \frac{d}{d\theta_{12}} (r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_{12})^{\frac{\mu-2}{2}} \right] \sin^2\theta_{12} d\theta_{12} \end{aligned}$$



which may be integrated once by parts to give

$$- \frac{2}{\mu-2} \frac{1}{r_1 r_2} \int r_{12}^{\mu-2} \cos \theta_{12} \sin \theta_{12} d\theta_{12}$$

and therefore

$$I = A(\nu+1, \lambda+1, \mu-2) + \frac{2}{\mu-2} B(\nu, \lambda, \mu)$$

from which it follows immediately that

$$B(\nu, \lambda, \mu) = \frac{\mu-2}{\mu+2} \left\{ B(\nu+2, \lambda, \mu-2) + B(\nu, \lambda+2, \mu-2) - 2A(\nu+1, \lambda+1, \mu-2) \right\} \quad (B-4)$$

## 2. Recursion Relations for $\mu = 1$ .

When  $\mu = 1$ , (B-1) becomes

$$A(\nu, \lambda, 1) = \int r_1^{\nu-2} r_2^{\lambda-2} F(r_1, r_2) \frac{1}{r_{12}} d\vec{r}_1 d\vec{r}_2.$$

Now recalling that in the coordinate system in use  $r_1 \geq r_2$ , so

$1/r_{12}$  can be expanded in a series of Legendre Polynomials

$$\frac{1}{r_{12}} = \sum_{\ell=0}^{\infty} \frac{r_2^{\ell}}{r_1^{\ell+1}} P_{\ell}(\cos \theta_{12})$$

and the angular integration becomes

$$\sum_{\ell=0}^{\infty} \frac{r_2^{\ell}}{r_1^{\ell+1}} \int_0^{\pi} P_{\ell}(\cos \theta_{12}) \sin \theta_{12} d\theta_{12} = \sum_{\ell=0}^{\infty} \frac{r_2^{\ell}}{r_1^{\ell+1}} \int_{-1}^1 P_{\ell}(u) du.$$

But  $P_0(u) = 1$  so the integral on the right can be rewritten

$$\int_{-1}^1 P_0(u) P_{\ell}(u) du$$

and by virtue of the orthogonality of the Legendre polynomials,

all terms in this expansion vanish except for  $\ell = 0$ . Therefore

$$A(\nu, \lambda, 1) = A(\nu-1, \nu, 2). \quad (B-5)$$



In a similar expansion in the case of  $B(v, \lambda, 1)$  all terms but  $\ell = 1$  vanish, giving

$$B(v, \lambda, 1) = \frac{1}{3} A(v-2, \lambda+1, 2). \quad (B-6)$$

### 3. Recursion Relations for $A_{s,c}(v, \lambda, \mu)$ and $B_{s,c}(v, \lambda, \mu)$

Referring to (53a)

$$A_s(v, \lambda, \mu) = A_1(v, \lambda, \mu) + A_2(v, \lambda, \mu)$$

and applying (B-3) above

$$\begin{aligned} A_s(v, \lambda, \mu) &= A_1(\lambda+2, v, \mu-2) + A_1(\lambda, v-2, \mu-2) - 2B_1(\lambda+1, v+1, \mu-2) \\ &\quad + A_2(v, \lambda+2, \mu-2) + A_2(v+2, \lambda, \mu-2) - 2B_2(v+1, \lambda+1, \mu-2) \\ &= A_s(v, \lambda+2, \mu-2) + A_s(v+2, \lambda, \mu-2) - 2B_s(v+1, \lambda+1, \mu-2) \end{aligned}$$

and similarly with  $B_s(v, \lambda, \mu)$ . Thus  $A_{s,c}$  and  $B_{s,c}$  satisfy the normal recursion relationships for  $\mu > 2$ . For  $\mu = 1$

$$\begin{aligned} A_s(v, \lambda, 1) &= A_1(\lambda, v, 1) + A_2(v, \lambda, 1) \\ &= A_1(\lambda-1, v, 2) + A_2(v-1, \lambda, 2) \end{aligned}$$

but

$$A_2(v-1, \lambda, 2) = A_s(v-1, \lambda, 2) - A_2(\lambda, v-1, 2)$$

so

$$A_{s,c}(v, \lambda, 1) = A_{s,c}(v-1, \lambda, 2) + A_{1,3}(\lambda-1, v, 2) - A_{1,3}(\lambda, v-1, 2) \quad (B-7)$$

where  $A_1$  is chosen when  $A_s$  is to be evaluated and  $A_3$  is chosen when  $A_c$  is to be evaluated. For  $B_{s,c}(v, \lambda, 1)$  the same procedure yields

$$B_{s,c}(v, \lambda, 1) = \frac{1}{3} \left\{ A_{s,c}(v-2, \lambda+1, 2) + A_{1,3}(\lambda-2, v+1, 2) - A_{1,3}(\lambda+1, v-2, 2) \right\} \quad (B-8)$$

which completes the derivation of all the relations needed to evaluate the matrix elements listed in Appendix A.





## APPENDIX C

### Rayleigh-Ritz Variational Method

Let an arbitrary quadratically integrable wave function  $\Psi$  be expanded in terms of the eigenfunctions of a bound system

$$\Psi = \sum_i a_i \chi_i \quad (C-1)$$

where

$$(H-E)\chi_i = 0$$

then on the function  $\Psi$  the expectation value of  $H$  is

$$\begin{aligned} \langle \Psi | H | \Psi \rangle &= \sum_{i,j} a_i^* a_j \langle \chi_i | H | \chi_j \rangle \\ &= \sum_i |a_i|^2 E_i \end{aligned} \quad (C-2)$$

If  $E_0$  is the ground state of the system, then  $E_0 \leq E_i$  so

$$E_0 \sum_i |a_i|^2 \leq \sum_i |a_i|^2 E_i$$

whence

$$\langle \Psi | H | \Psi \rangle \geq E_0$$

assuming

$$\langle \Psi | \Psi \rangle = 1$$

But

$$\langle \Psi | H | \Psi \rangle = E_\Psi$$

the expectation of  $H$  on  $\Psi$ , so if  $\Psi$  is found so as to minimize  $E_\Psi$  then  $E_\Psi \geq E_0$  and  $E_\Psi$  provides an upper bound on the value of  $E_0$ .



In general

$$E_{\Psi} = \langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle. \quad (C-3)$$

If now a trial wave function  $\Psi_t$  is chosen and expanded on a suitable basis  $\eta_i$

$$\Psi_t = \sum_{i=1}^N b_i \eta_i \xrightarrow{N \rightarrow \infty} \Psi \quad (C-4)$$

whence

$$E_t = \frac{\sum_{i,j} b_i^* b_j \langle \eta_i | H | \eta_j \rangle}{\sum_{i,j} b_i^* b_j \langle \eta_i | \eta_j \rangle} = \frac{\sum_{i,j} b_i^* b_j H_{ij}}{\sum_{i,j} b_i^* b_j S_{ij}}$$

where  $H_{ij} = \langle \eta_i | H | \eta_j \rangle$  and  $S_{ij} = \langle \eta_i | \eta_j \rangle$ . Now choosing the b's to satisfy

$$\frac{\partial E_t}{\partial b_i} = 0, \quad i = 1, \dots, N$$

gives

$$\frac{\partial E_t}{\partial b_i} \sum_{i,j} b_i^* b_j S_{ij} + E_t \frac{\partial}{\partial b_i} \sum_{i,j} b_i^* b_j S_{ij} = \frac{\partial}{\partial b_i} \sum_{i,j} b_i^* b_j H_{ij}$$

from which arise the N linear equations

$$\sum_i (H_{ij} - E_t S_{ij}) b_i = 0, \quad j = 1, \dots, N \quad (C-5)$$

which is just the first part of the Harris expansion technique, wherein the smallest eigenvalue  $E_t$  gives an upper bound on  $E_0$ .

The above method extends readily to the excited states [52]. This is achieved by choosing a trial wave function which is orthogonal to all the states lying below the desired one. Such a function must take the form

$$\Psi = \varphi - \sum_{n=0}^{N-1} X_n \langle X_n | \varphi \rangle \quad (C-6)$$



where  $\varphi$  is arbitrary and the  $\chi_n$  are the lower lying eigenstates. Then expanding  $\Psi$  according to (C-1) it is seen that the  $a_i$  are zero for  $i$  less than  $N$ , the index of the state desired, from which it follows that  $E_t \geq E_N$ .

Hylleraas and Undheim [32] have shown that this condition is automatically met by (C-5), the  $n^{\text{th}}$  eigenvalue of that equation being greater than or equal to the energy of the  $n^{\text{th}}$  level of the system. Thus it is seen that an important bonus in the Harris expansion method is a cataloging of the energy levels of the bound system formed by the scattering atom and the incident electron. Included in this cataloging are the autoionizing levels of the bound system which give rise to many of the observed scattering resonances [44].



## APPENDIX D

### Discussion of Numerical Calculations

#### 1. The Eigenvalue Problem

From Section II C.1, a solution for eigenvectors and eigenvalues is sought for the equation

$$(\underline{H} - \lambda \underline{S}) \vec{c} = 0 \quad (D-1)$$

Since  $\underline{S}$  is not the identity matrix (D-1) is not in the form usually associated with eigenvalue problems occurring in physics where the space is orthonormal and  $\underline{S}$  reduces to the identity matrix. This generalized eigenvalue problem has been extensively discussed in the mathematical literature [41]. In the present case, however, it is possible to reduce the problem to standard form and treat it by the simpler methods available.

Consider first the matrix  $\underline{S}$ . Its elements are the inner products of the chosen basis vectors

$$S_{ij} = \langle \chi_i | \chi_j \rangle \quad (D-2)$$

Since the basis functions are real  $S_{ij} = S_{ji}$  and therefore there exists a unitary transformation which diagonalizes  $\underline{S}$  [53], Physically this is equivalent to transforming to a new, orthogonal set of basis vectors. In this new set

$$S'_{ij} = \delta_{ij} \langle \chi'_i | \chi'_j \rangle$$





and  $S_{ii} > 0$  for all  $i$ .<sup>3</sup> But diagonalizing a matrix in this manner means that the new matrix has as its diagonal elements the eigenvalues of  $\underline{S}$ . Therefore it can be concluded that all the eigenvalues of  $\underline{S}$  are positive and hence  $\underline{S}$  is positive definite.

Now consider the positive definite quadratic form associated with  $\underline{S}$ ,  $\vec{x}^T \cdot \underline{S} \cdot \vec{x}$ . There exists a real non-singular transformation  $\underline{U}$  and a vector  $\vec{y}$  such that  $\vec{x} = \underline{U}^{-1} \cdot \vec{y}$  and such that (Ref. 53, p. 337)

$$\vec{y}^T \cdot \underline{U}^{-T} \cdot \underline{S} \cdot \underline{U}^{-1} \cdot \vec{y} = \vec{y}^T \cdot \vec{y} \quad (D-3)$$

called the "canonical form" of  $\vec{x}^T \cdot \underline{S} \cdot \vec{x}$ , where  $\underline{U}^{-T} = (\underline{U}^{-1})^T$ . Hence

$$\underline{U}^{-T} \cdot \underline{S} \cdot \underline{U}^{-1} = \underline{I} \quad (D-4)$$

where  $\underline{I}$  is the identity matrix. So

$$\underline{S} = \underline{U}^T \underline{U} \quad (D-5)$$

In other words, a positive definite symmetric matrix can always be factored into the product of a real non-singular matrix and its transpose. But because  $\underline{S}$  is symmetric, this factorization is not unique, for

$$S_{ij} = \sum_{k=1}^N U_{ki} U_{kj}$$

represents  $n^2$  equations, only  $n(n+1)/2$  of which are independent.

Therefore one is free to choose  $n(n-1)/2$  of the  $U_{\ell m}$  arbitrarily,

---

<sup>3</sup> Unless one of the new basis vectors is null, which would mean the dimensionality of the space is reduced - a possibility which can be excluded from the present problem.



and it is convenient to choose

$$U_{\ell m} = 0 \quad \ell > m$$

for then  $\underline{U}$  becomes an upper triangular matrix (one in which all elements below the principal diagonal are zero).

With the above choice of factorization of  $\underline{S}$ , (D-1) can be rewritten

$$\underline{U}^{-T} \cdot (\underline{H} - \lambda \underline{U}^T \cdot \underline{U}) \underline{U}^{-1} \cdot \underline{U} \cdot \vec{c} = 0$$

and the original problem reduces to

$$(\underline{U}^{-T} \cdot \underline{H} \cdot \underline{U}^{-1} - \lambda \underline{I}) \cdot \vec{x} = 0 \quad (D-6)$$

where  $\vec{x} = \underline{U} \cdot \vec{c}$ . Since  $\underline{H}$  is symmetric it is trivial to show  $\underline{U}^{-T} \cdot \underline{H} \cdot \underline{U}^{-1}$  is also symmetric, for

$$\begin{aligned} (\underline{U}^{-T} \cdot \underline{H} \cdot \underline{U}^{-1})_{mj} &= \sum_{i,k} U_{ik}^{-T} H_{ij} U_{ik}^{-1} = \sum_{i,k} U_{im}^{-1} H_{ki} U_{jk}^{-T} \\ &= \sum_{i,k} U_{jk}^{-T} H_{kj} U_{im}^{-1} = (\underline{U}^{-T} \cdot \underline{H} \cdot \underline{U}^{-1})_{jm} \end{aligned}$$

and the problem has been reduced to the standard problem of a real symmetric matrix in an orthonormal space.

The advantage of the form of the factorization of  $\underline{S}$  chosen is that because  $\underline{U}$  is triangular its inverse is particularly easy to obtain. The factorization is done by the square root method of Cholesky [54] and  $\underline{U}^{-1}$  is then found by solving the algebraic equations [55]

$$\left. \begin{aligned} U_{ii}^{-1} U_{ii} &= 1 \\ \sum_{j=1}^k U_{ij}^{-1} U_{jk} &= 0, \quad i < k \end{aligned} \right\} \quad i = 1, \dots, N \quad (D-7)$$

for the  $U_{ij}^{-1}$ .



Because the range of values of the elements of  $\underline{S}$  and  $\underline{H}$  was often several orders of magnitude (sometimes as many as fifteen or more) an additional check on the accuracy of  $\underline{U}^{-1}$  as found by the above method was used. If the  $\underline{U}^{-1}$  found above is taken as a first approximation to the exact inverse, then the following iteration scheme can be used to improve the value of the inverse [56].

Let  $\underline{C}_i$  be the  $i^{\text{th}}$  approximation to the exact inverse,  $\underline{U}^{-1}$ , and define the error matrix

$$\underline{R}_i = \underline{I} - \underline{C}_i \cdot \underline{U} . \quad (\text{D-8})$$

Then

$$\underline{C}_{i+1} = \underline{C}_i + \underline{R}_i \underline{C}_i = \underline{C}_i + (\underline{I} - \underline{C}_i \cdot \underline{U}) \cdot \underline{C}_i$$

and

$$\begin{aligned} \underline{R}_{i+1} &= \underline{I} - \{ \underline{C}_i + (\underline{I} - \underline{C}_i \cdot \underline{U}) \cdot \underline{C}_i \} \cdot \underline{U} \\ &= (\underline{I} - \underline{C}_i \cdot \underline{U})^2 = \underline{R}_i^2 \\ &= (\underline{R}_0^2)^i \end{aligned} \quad (\text{D-9})$$

where

$$\underline{R}_0 = \underline{I} - \underline{C}_0 \cdot \underline{U}$$

and  $\underline{C}_0$  is taken to be the value of  $\underline{U}^{-1}$  found by the Cholesky method above. Clearly, if the norm of  $\underline{R}_0$  is less than one the method converges quite rapidly, and since the value of  $\underline{C}_0$  is already quite accurate,  $\|\underline{R}_0\| \ll 1$ . In practice no more than one iteration of  $\underline{C}_0$  was ever required to make the elements of  $\underline{R}_i < 10^{-20}$ .

The eigenvalue problem was solved using the Jacobi variable threshold method [41,55]. This method proved to give the most accurate results although it is known to be considerably slower



than other methods tried. The accuracy of the eigenvalues was verified by the following method. For a given eigenvalue,  $\lambda_\mu$ , the determinant  $|\underline{H} - \lambda_\mu \underline{S}|$  was formed and compared with the determinant when  $\lambda_\mu$  was replaced by  $\lambda_\mu \pm \delta$  where  $\delta$  was typically  $10^{-7}$  (compared to  $\lambda_\mu$  which was on the order of one). Then  $\lambda_\mu$  was considered correct to six places if the respective determinants were related by

$$|\underline{H} - (\lambda_\mu \pm \delta) \underline{S}| < |\underline{H} - \lambda_\mu \underline{S}| < |\underline{H} - \lambda_\mu \mp \delta) \underline{S}| \quad (\text{D-10})$$

and the first and last terms above were of opposite sign. Accuracy of the eigenvectors was not so clearly established, though a similar procedure to the above was followed. The product  $(\underline{H} - \lambda_\mu \underline{S}) \vec{c}$  was formed and it was noted that as  $\lambda$  was perturbed as above, all elements in the resultant vector changed sign. While this indicated that the eigenvectors probably are reasonably accurate no quantitative bound could be placed on their error. Further indication of the accuracy of the eigenvectors can be inferred from the close agreement of the phase shift results for hydrogen with the accepted values found by Schwartz [12].

## 2. Numerical Integration

From the beginning it was felt that the simplest and most reliably accurate means of evaluating the necessary integrals numerically would be some form of Gaussian quadrature [57]. Any numerical integration scheme attempts to replace the integration by a finite sum so chosen as to make the error tolerably small

$$\int_a^b f(x) dx \approx \sum_{i=0}^n w_i f(x_i) \quad (\text{D-11})$$





where the  $w_i$  are weights to be assigned to the function evaluated at the sampling points  $x_i$ , in other words a weighted average of the function at the various sample points. If the  $x_i$  are fixed, equally spaced points then the  $n + 1$   $w_i$  can be chosen to define a polynomial of order  $n$  with which to approximate  $f(x)$ , and if  $f(x)$  is itself a polynomial of order  $n$  or less, the integration will be exact. If however, one is free to vary the  $x_i$  also, there will now be  $2n + 2$  parameters available and it will be possible to define a polynomial of degree  $2n + 1$  with which to approximate  $f(x)$ . Thus, given the values of  $x_i$  and  $w_i$  in each case, the same amount of labor results in a more accurate integration in the second case.

Adopting this approach, one can approximate  $f(x)$  with a Lagrangian interpolating polynomial of degree  $(n + 1)$  of the form

$$f(x) = g(x)F(x) = \sum_{i=0}^n L_i(x)g(x)F(x_i) + R_n(x) \quad (D-12)$$

where

$$L_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^n \frac{(x - x_j)}{(x_i - x_j)} \quad (D-13)$$

and  $R_n(x)$  is the remainder term, given by

$$R_n(x) = \prod_{i=0}^n (x - x_i) F^{(n+1)}(\xi) g(x) / (n+1)!, \quad a < \xi < b \quad (D-14)$$

The reason for factoring  $f(x)$  into  $g(x)F(x)$  will become apparent below. Now if  $F(x)$  is a polynomial of degree  $2n + 1$  then  $F^{(n+1)}(\xi)$  must be a polynomial of degree  $n$ . Letting

$$\frac{F^{(n+1)}(\xi)}{(n+1)!} = q_n(x)$$



where  $q_n(x)$  is a polynomial of degree  $n$ , (D-14) becomes

$$R_n(x) = q_n(x) \prod_{i=0}^n (x-x_i) g(x) \quad (D-15)$$

Integrating (D-12) gives

$$\int_a^b g(x) F(x) dx = \sum_{i=0}^n F(x_i) \int_a^b g(x) L_i(x) dx + \int_a^b g(x) q_n(x) \prod_{i=0}^n (x-x_i) dx \quad (D-16)$$

Now (D-16) is of the form (D-11) where

$$w_i = \int_a^b g(x) \prod_{\substack{j=0 \\ j \neq i}}^n \frac{(x-x_j)}{(x_i-x_j)} dx \quad (D-17)$$

except that the  $x_i$  have not been chosen. The object is to so choose the  $x_i$  that the second term of (D-16) vanishes. This is easily done if  $q_n(x)$  and  $\prod_{i=0}^n (x-x_i)$  are expanded in a series of polynomials orthogonal on  $[a,b]$  with respect to the weight function  $g(x)$ . A weight function appropriate to a particular set of orthogonal polynomials is often a natural factor in the function to be integrated and therefore the particular expansion to be chosen may be dictated by the problem, hence the utility in carrying the factor  $g(x)$  through the derivation.

Let the polynomials chosen for the expansion be designated  $P_n(x)$  whereupon

$$\prod_{i=0}^n (x-x_i) = \sum_{\ell=0}^{n+1} b_\ell P_\ell(x) \quad (D-18)$$

and

$$q_n(x) = \sum_{m=0}^n c_m P_m(x) \quad (D-19)$$



Combining these two expansions in (D-15) and applying the orthogonality condition

$$\int_a^b g(x) P_\ell(x) P_m(x) dx = 0, \quad \ell \neq m \quad (D-20)$$

reduces the error term to

$$\int_a^b g(x) q_n(x) \prod_{i=0}^n (x-x_i) dx = \sum_{j=0}^n b_j c_j \int_a^b g(x) [P_j(x)]^2 dx \quad (D-21)$$

Now if the  $x_i$  are chosen to be the zeroes of  $P_{n+1}(x)$ , then the expansion (D-18) reduces to

$$\prod_{i=0}^n (x-x_i) = b_{n+1} P_{n+1}(x)$$

i.e.,  $b_j = 0 \quad 0 \leq j \leq n$ , whence (D-21) vanishes, and the integration is exact. Thus evaluating the function at  $n+1$  carefully chosen points suffices to integrate it exactly if it can be expressed in terms of a polynomial of degree  $2n + 1$  or less, a considerable improvement over the equally spaced interval methods, as was promised above. The one remaining problem is, then, to evaluate the  $w_i$ 's and find the  $x_i$ 's. Fortunately, this has been done for a large class of orthogonal polynomials by Stroud and Secrest [58].

Although the integration limits and the form of the integrands (49), (51), (56) and (57) suggest the use of the Laguerre polynomials for the numerical integrations, the almost periodic nature of the functions and the ever increasing amplitude in the absence of the  $e^{-x}$  factor dictated the use of a finite interval formula where several intervals could be integrated separately and then added together to give the final result. Since the factor  $e^{-x}$  forces the integral to zero at large  $x$ , examination of the integrands



indicated that an upper limit on the integration of  $x = 100$  would introduce a negligible error from the neglected region in the worst possible case. Because the variable change to conform to the convergence limits of the polynomials used in the expansions (D-18,19) is simple and because the weight function is unity the decision was made to use Legendre polynomials in the integration.

Because of the almost periodic nature of the integrands, when the instantaneous frequency of the sinusoidal variation is large the areas under the integrand above and below the axis are nearly equal and substantial loss of significance occurs when these two values are subtracted. Often as many as eight to twelve significant figures can be lost due to subtraction, hence great care must be taken to avoid the problem. The approach adopted was to seek a function whose exact integral is known and which approximates the desired integral closely enough so that the difference between them is small, then evaluating this small difference numerically and adding the result to the known value of the approximating function. This method can be compared to the measurement of the difference between two large quantities, say frequencies. Often the difference can be determined quite accurately even though the absolute magnitude is known only approximately.

In executing this approach to the integration of the functions at hand the first step is to find all the zeroes of the integrand between arbitrarily chosen minimum and maximum values of  $x$ . These values are then used as the end points of the subintervals in an integration of the form

$$I(x) = \int_0^{z_1} f(x) dx + \sum_{i=1}^n \left\{ \int_{z_i}^{z_{i+1}} [f(x) - h_i(x)] dx + \int_{z_i}^{z_{i+1}} h_i(x) dx \right\} + \int_{z_{n+1}}^{100} f(x) dx \quad (D-22)$$





where the  $z_i$  are the  $n + 1$  zeroes of  $f(x)$  found above and the  $h_i(x)$  are functions whose exact integral is known and which approximate  $f(x)$  over the interval indicated. The  $h_i(x)$  are chosen as indicated in Figure 23. Note that  $h_i(x)$  is amplitude modulated from segment to segment so that  $f(x) - h_i(x)$  is always mostly positive and smaller than  $f(x)$  by at least an order of magnitude regardless of the sign of  $f(x)$ . It is this difference function which is integrated numerically, and since  $h_i(x)$  is a different function for each half cycle of  $f(x)$  the numerical integration is done in segments between zeroes of the function using a 32-point Gauss-Legendre quadrature on each segment.

The form chosen for  $h_i(x)$  was

$$h_i(x) = (1 + \frac{p}{10}) \sin(A_x + B) e^{-x} x^\gamma (1 - e^{-\beta x})^3 \quad (D-23)$$

where  $p$  is  $+1$  if  $f(x)$  is negative and  $-1$  if  $f(x)$  is positive,  $\beta = 1$  if  $I_s$  or  $I_c$  is to be found and  $\beta = \alpha/2(Z+\alpha)$  if  $I_1$  or  $I_3$  is to be found, and

$$A = \frac{\pi}{z_{i+1} - z_i}, \quad B = A \left[ \left(1 + \frac{1-p}{2}\right) z_{i+1} - \left(2 + \frac{1-p}{2}\right) z_i \right] \quad (D-24)$$

so chosen that  $\sin(Ax + B)$  vanishes at the end points of each segment and nowhere in between.

When chosen in this manner the integral of  $h_i(x)$  alone is exact and has a rather simple form. If  $(1 - e^{-\beta x})^3$  is expanded four integrals of the form

$$S_\ell = \int_{z_i}^{z_{i+1}} \sin(A_x + B) e^{-a_\ell x} x^\gamma dx, \quad \ell = 1, 2, 3, 4 \quad (D-25)$$



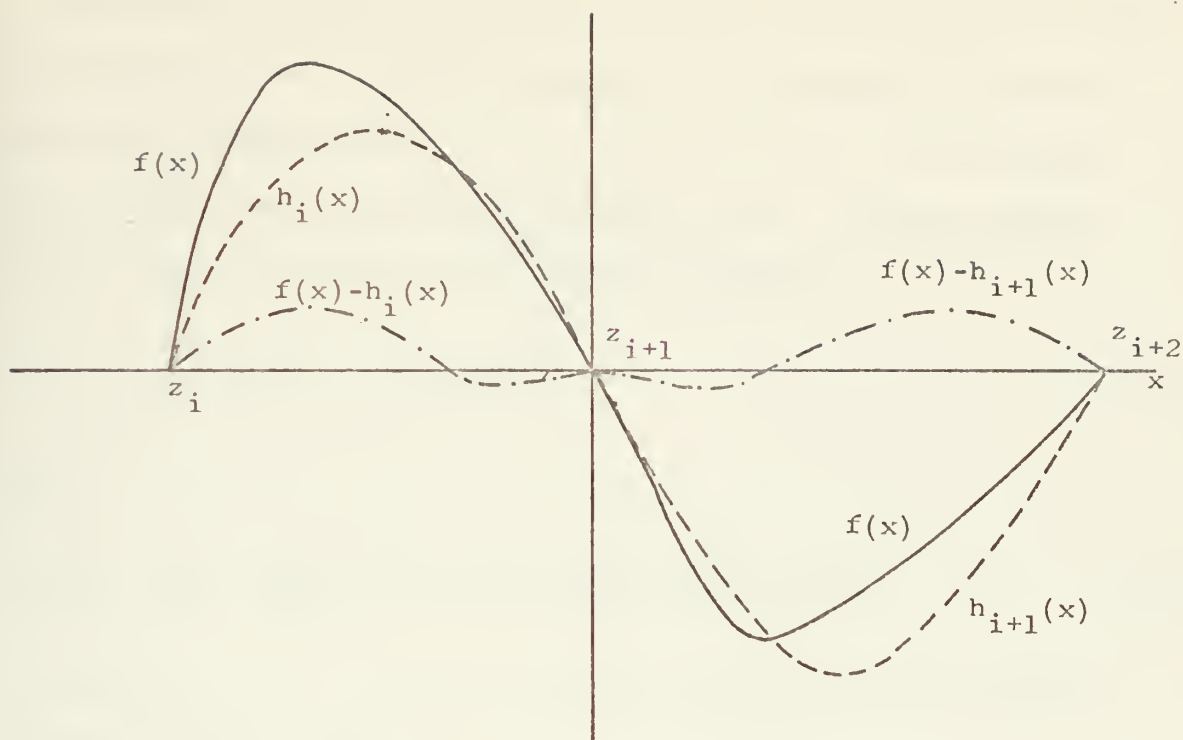


Figure 23.

Example of Method of Choosing  $h_i(x)$

result, where  $a_\ell$  is  $1, 1 + \beta, 1 + 2\beta$  and  $1 + 3\beta$  in turn. These integrate immediately to

$$S_\ell = \gamma! \sum_{j=1}^{\gamma+1} \frac{\sin(j\theta)}{(-\rho)^j (\gamma+1-j)!} \left( e^{-a_\ell z_{i+1}} z_{i+1}^{\gamma+1-j} + e^{-a_\ell z_i} z_i^{\gamma+1-j} \right) \quad (D-26)$$

where  $\theta$  and  $\rho$  satisfy the relationship

$$-a + (-1)^{\frac{1}{2}} A = \rho (\cos\theta + (-1)^{\frac{1}{2}} \sin\theta)$$

and finally

$$\int_{z_i}^{z_{i+1}} h_i(x) dx = P \left( 1 + \frac{P}{10} \right) (S_1 - 3S_2 + 3S_3 - S_4) \quad (D-27)$$



Expressions (D-26,27) are valid for  $\gamma \geq 0$ . During the course of evaluating the phase shifts, however, it is necessary to evaluate the various integrals for  $\gamma = -1$ . For this case a slightly different scheme must be used to evaluate  $h_i(x)$ . If one replaces  $(1 - e^{-\beta x})/x$  in (D-23) by the integral identity

$$\frac{1 - e^{-\beta x}}{x} = \beta \int_0^1 e^{-\beta xy} dy \quad (D-28)$$

then

$$h_i(x) = \beta \left(1 + \frac{p}{10}\right) \int_0^1 \sin(Ax+B) e^{-x} (1 - e^{-\beta x})^2 e^{-\beta xy} dy \quad (D-29)$$

Carrying out the  $x$  integration first and making the appropriate variable changes yields

$$S_\ell = \int_{\beta\ell+1}^{\beta(\ell+1)+1} \frac{e^{-z_i w} + e^{-z_{i+1} w}}{w^2 + A^2} dw \quad (D-30)$$

and finally

$$\int_{z_i}^{z_{i+1}} h_i(x) dx = -P \left(1 + \frac{p}{10}\right) \cdot A \cdot (S_0 - 2S_1 + S_2) \quad (D-31)$$

Unfortunately (D-30) must be integrated numerically also, however it is a relatively slowly varying function of  $w$  and is always positive so integration by a 32-point Gauss-Legendre quadrature gives more than adequate accuracy.

To complete the integration of (D-22) the first and last terms were evaluated using single 512-point Gauss-Legendre quadratures.

Since the accuracy of the numerical integration is crucial to the accuracy of the phase shifts calculated for helium ion scattering, a great deal of effort was expended to insure that the methods were both correct and internally accurate.



The first and most obvious check is to increase the number of sample points in the numerical integrations. This was done by increasing the quadrature method on each interval to 64 points. Changes to the integrals on doing this were typically in the 12<sup>th</sup> to 14<sup>th</sup> digit, indicating that the differences were principally due to round-off error since the maximum number of digits available was 16.

The integration scheme described above grew out of a similar method which was used extensively prior to the present one for the same calculations. The present method was adopted in an effort to extend the useable range of the parameters involved in the integrands. The problems with the former method arose principally because it was not sufficiently accurate when the oscillation frequency of the sinusoidal function was high. However in the region where both schemes were adequate (which proved to be almost everywhere) the integrals were consistently reproduceable to 12 to 14 places. The choice of integration intervals and of the  $h_i(x)$  in the earlier method was sufficiently different that it constitutes an almost independent check on the internal accuracy of the integrals.

Three different methods were used to make the integrals exactly integrable so that the numerical results could be compared directly with known answers and to provide a check on the correctness of the expressions. The first was to let  $k \rightarrow \infty$  while holding the ratio  $k/\alpha$  constant. This forces the logarithmic terms to zero and reduces the integral to a standard form which can be integrated directly. The direct evaluation was done on a Hewlett-Packard





Model 9810A computer which gave results to ten significant figures. These results were then compared with the numerical results and except in the cases where  $k/\alpha$  was at its extreme limits, agreement was obtained to eight to ten places. This method was tried only with the older integration scheme and so some decay at the limits of  $k/\alpha$  was expected. In addition, the transition from the form of the integral when  $k$  was finite to its form as  $k \rightarrow \infty$  appeared smooth and with no obvious discontinuities or other strange behavior in the transition region.

A second check took advantage of the fact the computer program was written to allow for variation of the nuclear charge,  $Z$ . Although the intent was to limit the value of  $Z$  to integers, nothing in the program or the mathematics forbade varying the charge continuously from one to two. When this was done, it was again seen that the result for  $Z = 2$  transitioned smoothly into that for  $Z = 1$  with no discontinuities as the charge was varied.

Since for  $Z = 1$  the integrals all become exactly integrable, the computer program did not do the calculations required for the numerical integration in the case of  $Z = 1$ , but skipped to a subroutine which evaluated directly the exact integrals. The final comparison method was to circumvent the exact integration routine for  $Z = 1$  and do these integrals numerically, using the method described at length above. Again the agreement between the two calculations was excellent, the integrals and the phase shifts typically being identical in the first twelve to fifteen places.



The final check was to test the sensitivity of the entire calculation to perturbations in  $k$ . It was noted that even at the extreme limits of  $k/\alpha$  where accuracy was expected to be poorest, only some of the integrals showed evidence of loss of significance from the subtraction problem mentioned above. For these integrals, however, a small perturbation in the value of  $k$  may have a relatively large effect on the integration and if the inaccurate integrals dominated the computation then they could significantly distort the results. As before when this perturbation was artificially fed into the problem its effect was well within the limits considered acceptable (results unchanged to six places or more for a perturbation of  $k$  in the seventh place) except at the extremes.

Since none of these tests indicate any serious problems with accuracy it is felt that the errors inherent in numerical integration have been kept well within tolerable bounds in this problem and the results can be relied upon with considerable confidence. It also proved to be true that those regions where accuracy was lost were easily avoidable.

### 3. Evaluation of $\Gamma(1 - ia)$

From the definition of the gamma function

$$\Gamma(P) = \int_0^{\infty} e^{-x} x^{P-1} dx \quad (D-32)$$

one finds

$$\Gamma(1-ia) = \int_0^{\infty} e^{-x} x^{-ia} dx \quad (D-33)$$

but  $e^{\ln(x)} = x$ , so (D-33) can be rewritten

$$\begin{aligned} \Gamma(1-ia) &= \int_0^{\infty} e^{-x} \cos(a \ln x) dx - i \int_0^{\infty} e^{-x} \sin(a \ln x) dx \\ &= A + iB \end{aligned} \quad (D-34)$$



whence

$$\arg \{ \Gamma(i-ia) \} = \tan^{-1} \frac{B}{A} \quad (D-35)$$

and the evaluation of the complex gamma function is reduced to evaluating two real integrals. The integrals have to be evaluated numerically, however, and are not suitable for this in the form (D-34) because the rapid oscillations of the integrand near the origin could contribute to a substantial error in the numerical integration. To overcome this problem note that an integration by parts of each of the integrals (D-34) introduces a factor  $x$  into the integrand and this has the desirable effect of reducing the contribution of the integrand near the origin. Each repetition of the partial integration introduces an additional factor of  $x$  into the integrand. Carrying out this process three times transforms the integrals (D-34), after considerable algebra, into

$$B = \frac{-a}{(1+a^2)(4+a^2)(9+a^2)} \int_0^\infty x^3 e^{-x} \left\{ \frac{6}{a} (a^2-1) \sin(ax) - (a^2-11) \cos(ax) \right\} dx \quad (D-36)$$

and

$$A = \frac{-a}{(1+a^2)(4+a^2)(9+a^2)} \int_0^\infty x^3 e^{-x} \left\{ (a^2-11) \sin(ax) + \frac{6}{a} (a^2-1) \cos(ax) \right\} dx \quad (D-37)$$

which forms are now quite suitable for numerical integration.

The integrations of these functions were carried out using a 256-point Gauss-Legendre quadrature over 15 arbitrarily chosen intervals. To check accuracy the results were compared with another program which calculated the complex gamma function using a Pade-power approximation method and claimed 9-place accuracy.



The internal accuracy of the integration scheme was checked by comparing the 256-point integrations to 512-point integrations on the same intervals. This comparison indicated accuracy to about 13 places and these results were consistent with those found by the comparison program. In addition the numerical integrations seemed to take somewhat less time than was required by the power series method and was not subject to slow convergence as the imaginary part of the argument became large.





# COMPUTER PROGRAM

PROGRAM PHASE        MK IV        SEPT 1972

IMPLICIT REAL\*8 (A-H,O-Z)

INTEGER RO

EXTERNAL CGARG,FACT,DCOS,DSIN,FQN,FCN

STORAGE FOR SAMPLE POINTS AND WEIGHTS FOR 256 AND 512 POINT  
GAUSS-LEGENDRE INTEGRATIONS.

COMMON/L256/X256(128),A256(128)

COMMON/L512/X512(256),A512(256)

INTEGRATION INTERVALS FOR GAMMA FUNCTION INTEGRATIONS

COMMON/CD/DPC(15),DMC(15)

MISCELLANEOUS CONSTANTS USED IN VARIOUS SUBROUTINES

COMMON/CONST/PH1,PH2,FR1,FR2,ASCL,P1,CA,CT,AA

PASSES ALPHA AND AND ETA TO THE INTEGRATION AND MATRIX ROUTINES

COMMON/TRM/ALFA,ETA

PASSES K TO THE INTEGRATION ROUTINE

COMMON/WAVP/WAVN

PASSES NUCLEAR CHARGE

COMMON/ATNO/Z

DUMMY VARIABLES. THIS COMMON USED IN INTEGRATIONS FOR  
RHO = - 1

COMMON/MCNE/D1,D2,D3

USED IN DETERMINING THE LIMITS OF THE RANGE OF THE INTEGRAND  
OVER WHICH TO FIND THE ZEROES

COMMON/INT/XSM,FF,BJ,XLM

DUMMY VARIABLES. THIS COMMON USED IN INTEGRATIONS FOR  
RHO > -1

COMMON/GEZRO/D4,D5,D6,I10,I20



INDICES FOR MATRIX ELEMENTS

COMMON/INDEX/NI,NJ,LI,LJ,MI,MJ,IS

VALUE OF EXPONENT OF X IN BOUND-FREE INTEGRALS

COMMON/RHO/RO

STORAGE FOR BOUND-FREE INTEGRALS

DIMENSION AS(1452),BS(1452),AC(1452),BC(1452)

STORAGE FOR THE VALUES OF THE EXPONENTS OF R1, R2 AND R12 IN THE HYLLERAAS FUNCTIONS. LOCATION OF THE REGIONS OF ALPHA TO BE SKIPPED IN THE CALCULATION

DIMENSION N(95),L(95),M(95),ISTP(10)

DATA INPUTS FOR EXACT ENERGY CALCULATIONS

DIMENSION X(5),Y(5)

C DIMENSION STATEMENTS FOR PHASE SINGLET, N=7.

STORAGE FOR BOUND-BOUND INTEGRALS

DIMENSION A(5508),B(5508)

STORAGE FOR MATRIX ELEMENTS AND EIGENVECTOR ELEMENTS

DIMENSION H(70,70),S(70,70),C(70,70)

STORAGE FOR EIGENVALUES

DIMENSION WAV(70),ENERG(70)

STORAGE FOR UPPER TRIANGULAR ELEMENTS OF H AND S AND FOR THE INVERSE OF THE TRIANGULAR FACTOR OF S

DIMENSION TH(2485),TS(2485)

EQUIVALENCE(H(1),AS(1)),(H(2451),BS(1))

EQUIVALENCE(S(1),AC(1)),(S(2451),BC(1))

C

DATA FOR THE HYLLERAAS FUNCTIONS AND THE NUMERICAL INTEGRATIONS ARE STORED IN A SEQUENTIAL DATA SET

READ(8,1000)N,L,M

READ(8,1002) DPC,DMC

READ(8,1001)(X512(II),A512(II),II=1,256)

READ(8,1001)(X256(KK),A256(KK),KK=1,128)

REMAINDER OF DATA FOR PRESENT CALCULATION IS READ IN FROM PUNCHED CARDS SUBMITTED WITH THE MAIN PROGRAM. THIS DATA REMAINS FIXED FOR THE ENTIRE PROGRAM: INDEX FOR NUMBER OF INTEGRATIONS, TOTAL SPIN, BASIS SET SIZE DETERMINED BY THIS



INDEX, NUMBER OF ENERGIES TO BE INVESTIGATED (SET THIS EQUAL  
TO ONE IF THE ENTIRE ELASTIC RANGE IS TO BE COVERED),  
NUCLEAR CHARGE

READ(5,1021) NSET,IS,MATRIX,INO,Z

IF(IS.EQ.0) GO TO 88

IF TOTAL SPIN IS ONE (TRIPLET) SCREEN OUT THOSE FUNCTIONS  
NOT NEEDED FOR THE CALCULATION

K = 0

DO 100 KK=1,95

IF(N(KK).EQ.L(KK)) GO TO 100

K = K + 1

N(K) = N(KK)

L(K) = L(KK)

M(K) = M(KK)

IF(K.EQ.MATRIX) KK = 95

100 CONTINUE

SET VARIOUS CONSTANTS WHICH DETERMINE NEEDED INTEGRALS

88 MAX = 2\*NSET + 4

IMAX = NSET + 5

MAXI = NSET + 3

LIM = MATRIX\*MATRIX

ISIZE = MATRIX\*(MATRIX + 1)/2

FIND THE REQUIRED BOUND-BOUND INTEGRALS

CALL TBL1(MAX,A,B)

SET CONSTANTS NEEDED FOR THE NUMERICAL INTEGRATIONS

PI = 0.3141592653589793D1

XSM = 0.5D-2

FF = 0.3D-1

B0 = 0.16D2

XLM = 0.455D2

FIRST LOOP. READ DATA FOR THE RANGE OF ALPHA AND ENERGY TO  
BE INVESTIGATED.

DO 130 IW=1,INO

READ(5,1008) IALO,IAHI,IAINT,NUM,FCT,PLO,PHI

VALUES OF ALPHA TO BE SKIPPED

READ(5,1005) ISTP



USED TO LIMIT SEARCH FOR CLOSEST EIGENVALUES IN EXACT ENERGY CALCULATIONS. IF NO EIGENVALUE IS FOUND WITHIN THIS EXTENDED RANGE THE CALCULATION IS STOPPED FOR THAT ENERGY

PHIEXT = PHI + 0.1D-1

PLDEXT = PLD - 0.1D-1

SECOND LOOP. COVERS DESIRED RANGE OF ALPHA FOR DESIGNATED ENERGY

102 DO 101 IA=IALO,IAHI,IAINT

IF THE LOW VALUE OF K DESIRED IS ZERO, THE ENTIRE ELASTIC SCATTERING REGION WILL BE INVESTIGATED. SKIP THE EXACT ENERGY CALCULATION

IF(PLD.EQ.0.0D0) GO TO 50

READ THE VALUES OF ALPHA AND K FOR THE FIVE POINTS ON THE TRAJECTORY CLOSEST TO THE DESIRED VALUE OF K

READ(5,1016)(Y(I),X(I),I=1,5)

XINT = PLD + 0.5D-6

USING A CUBIC INTERPOLATING POLYNOMIAL, FIND AN ESTIMATE OF THE VALUE OF ALPHA REQUIRED TO GIVE THE DESIRED VALUE OF K

70 CALL SPLIN1(X,Y,5,XINT,YINT)

ALFA = YINT

GO TO 51

CHECK TO SEE IF A SEGMENT OF THE ALPHA RANGE IS TO BE SKIPPED. NOT USED WHEN THE EXACT ENERGY CALCULATION IS USED

50 DO 103 I=1,NUM,2

IF (IA.EQ.ISTP(I)) IA=ISTP(I+1)

103 CONTINUE

ALFA = FCT\*DFLOAT(IA)

EVALUATE THE H AND S MATRIX ELEMENTS

51 DO 16 J=1,MATRIX

JJ = J\*(J - 1)/2

DO 10 I=1,J

NI = N(I)

NJ = N(J)

LI = L(I)

LJ = L(J)

MI = M(I)

MJ = M(J)





```

CALL ELEM(HH,SS,A,B,MAX)
IJ = I + JJ
H(I,J) = HH
TH(IJ) = HH
S(I,J) = SS
10 TS(IJ) = SS
16 CONTINUE

BEFORE FACTORING S, SCALE IT SO THE LARGEST ELEMENT IS < 10.
F IS THE SCALE FACTOR
CALL SCL(TS,ISIZE,F)
WRITE(6,1006) F
CALL SMPY(TS,F,ISIZE)

FACTOR S INTO ITS TRIANGULAR ELEMENTS AND INVERT THE UPPER
TRIANGULAR FACTOR. RETURN IT IN TS
CALL INVERT(TS,H,S,C,MATRIX,ISIZE)

FORM U**(-T)*H*U**(-1). RETURN IT IN TH
CALL TMPRD(TH,TS,C,MATRIX,F)

EXPAND TH TO FULL SIZE AND STORE IN H. PUT TS IN UPPER
TRIANGLE OF S AND SAVE FOR FUTURE USE
DO 20 J=1,MATRIX
JJ = J*(J - 1)/2
DO 20 I=1,J
IJ = I + JJ
HT = H(I,J)
H(I,J) = TH(IJ)
H(J,I) = TH(IJ)
TH(IJ) = HT
S(J,I) = 0.000
20 S(I,J) = TS(IJ)
TRACE = 0.000
DO 11 I=1,MATRIX
11 TRACE = TRACE + H(I,I)
WRITE(6,1013) TRACE

FIND EIGENVALUES AND EIGENVECTORS OF TRANSFORMED H MATRIX
CALL DJACVT(H,MATRIX,1,ENERG,C,MATRIX)

```



TRACE = 0.000

FIND SUM OF EIGENVALUES AND COMPARE WITH TRACE OF H PREVIOUSLY FOUND

DO 17 I=1,MATRIX

17 TRACE = TRACE + ENERG(I)

WRITE(6,1015) TRACE

SCALE EIGENVECTORS SO LARGEST ELEMENT IS < 10

CALL SCL(C,LIM,F)

CALL SMPY(C,F,LIM)

MULTIPLY THE ORTHOGONAL EIGENVECTORS BY U\*(-1) TO FIND THE EIGENVECTORS OF THE ORIGINAL PROBLEM

CALL MPRD(S,C,H,MATRIX)

WRITE(6,3002) ALFA

WRITE(6,3004) ENERG

IK = 0

THIRD LOOP. EXAMINE THE EIGENVALUES TO FIND THOSE IN THE DESIRED ENERGY RANGE

DO 15 IE=1,MATRIX

WAV(IE) = 0.000

E = ENERG(IE)

ROOT = 0.2D17 \* E + Z \* Z

IF(ROOT.LE.0.000) ROOT = 0.000

PINT = DSQRT(ROOT)

IF((PINT.LE.PLO).OR.(PINT.GT.PHI))GO TO 21

INDEX GIVING NUMBER OF EIGENVECTORS IN THE DESIRED ENERGY RANGE

IK = IK + 1

WAV(IK) = PINT

EIGENVALUES IN DESIRED RANGE RELOCATED IN FIRST ADDRESSES OF EIGENVALUE VECTOR

ENERG(IK) = E

EIGENVECTOR CORRESPONDING TO ABOVE EIGENVALUE RELOCATED IN APPROPRIATE COLUMN OF EIGENVECTOR MATRIX

DO 12 K=1,MATRIX

12 C(K,IK) = C(K,IE)



IN EXACT ENERGY CALCULATION ASSUME FIRST VALUE WITHIN  
DESIRED LIMITS THE ONE LOOKED FOR

IF(PLO.GT.0.000) IE = MATRIX

GO TO 15

IF EXACT ENERGY FEATURE IS NOT BEING USED SKIP THIS SECTION

21 IF(PLO.EQ.0.000) GO TO 15

IF EIGENVALUE BEING EXAMINED IS OUTSIDE THE EXTENDED RANGE  
GO ON TO THE NEXT ONE

IF((PINT.LT.PLOEXT).OR.(PINT.GT.PHIEXT))GO TO 15

IF EIGENVALUE IS OUTSIDE THE DESIRED RANGE BUT WITHIN THE  
EXTENDED ONE, PRINT THE VALUE AND REPLACE THE OUTERMOST  
POINT ON THE SEGMENT OF THE TRAJECTORY UNDER EXAMINATION BY  
THIS VALUE. THEN GO BACK AND RECALCULATE AN IMPROVED  
ESTIMATE OF THE REQUIRED ALPHA

WRITE(6,1014) IE,PINT

KNUM = 0

IF(PINT.LT.X(1)) KNUM = 1

IF(PINT.GT.X(5)) KNUM = 5

IF((KNUM.EQ.1).OR.(KNUM.EQ.5)) GO TO 65

DO 60 I=2,5

IF((PINT.LT.X(I)).AND.(PINT.GT.X(I-1))) KNUM = I

60 CONTINUE

IF((KNUM.LT.1).OR.(KNUM.GT.5)) GO TO 15

IF((PINT-X(1)).GE.(X(5)-PINT)) GO TO 61

DO 62 I=1,4

IL = 5 - I

IF(IL.GE.KNUM) X(IL+1) = X(IL)

IF(IL.GE.KNUM) Y(IL+1) = Y(IL)

62 CONTINUE

X(KNUM) = PINT

Y(KNUM) = ALFA

GO TO 70

61 KNUM = KNUM - 1

DO 63 I=2,5

IF(I.LE.KNUM) X(I-1) = X(I)

IF(I.LE.KNUM) Y(I-1) = Y(I)

63 CONTINUE

65 X(KNUM) = PINT



```

Y(KNUM) = ALFA
GO TO 70
15 CONTINUE

```

IF NO EIGENVALUES WERE FOUND IN THE DESIRED RANGE, GO TO THE NEXT VALUE OF ALPHA

```

IF(IK.EQ.0) GO TO 101
WRITE(6,3005) ALFA
WRITE(6,3004)(WAV(LP),LP=1,IK)

```

FOURTH LOOP. BEGIN THE PHASE SHIFT CALCULATION

```

DO 113 NN=1,IK
E = ENERG(NN)
WAVN = WAV(NN)

```

FIRST FIND THE COULOMB PHASE SHIFT, ETA

```

AA = (Z - 0.1D1)/WAVN

```

IF Z = 1 SKIP THIS PART AND GO ON TO THE BOUND-FREE INTEGRATIONS

```

IF(AA.EQ.0.0D0) GO TO 301
ASQ = AA*AA
CA =ASQ - 0.11D2
CT = 0.6D1*(ASQ - 0.1D1)/AA
CALL INT256(C3ARG,GR)
CA = CT
CT= 0.11D2 -ASQ
CALL INT256(C3ARG,G1)
GR = -GR
ETA = DATAN2(G1,GR)
GO TO 302

```

```

301 ETA = 0.0D0

```

```

WRITE(6,1020) MATRIX,MATRIX,ALFA,E,WAVN
GO TO 303

```

```

302 WRITE(6,1004) MATRIX,MATRIX,ALFA,E,WAVN,ETA,Z

```

FIND THE REQUIRED BOUND-FREE INTEGRALS

```

303 CALL TBL2(IMAX,MAXI,AS,AC,BS,BC)
STERM = 0.0D0
CTERM = 0.0D0

```





FORM THE BOUND-FREE MATRIX ELEMENTS

DO 300 JM=1,MATRIX

CC = C(JM,NN)

NJ = N(JM)

LJ = L(JM)

MJ = M(JM)

CALL PHASE(AS,AC,BS,BC,MAXI,HS,HC,E)

HSC = HS\*CC

STERM = STERM + HSC

HCC = HC\*CC

CTERM = CTERM + HCC

300 CONTINUE

EVALUATE THE PHASE SHIFT

TDLTA = -STERM/CTERM

TDLTAK = TDLTA/WAVN

DLTA = DATAN(TDLTA)

IF(IS.EQ.0) GO TO 91

WRITE(6,1011)

GO TO 92

91 WRITE(6,1012)

92 WRITE(6,1007) ALFA,WAVN,TDLTA,TDLTAK,DLTA

WRITE(7,1100) ALFA,WAVN,TDLTA,TDLTAK,DLTA

IF(DLTA.GT.0.000) GO TO 113

IF THE PHASE SHIFT IS NEGATIVE, ARBITRARILY ADD PI TO IT AND  
PRINT AN ADDITIONAL DATA CARD WITH THE NEW PHASE SHIFT

DLTAP = DLTA + PI

WRITE(7,1101) ALFA,WAVN,DLTAP

113 CONTINUE

101 CONTINUE

130 CONTINUE

STOP

1000 FORMAT(48I1,/,47I1)

1001 FORMAT(2D30.16)

1002 FORMAT(8D9.3,/,7D9.3)

1003 FORMAT('-',5X,'SOLUTIONS FOR ALPHA =',F11.6,/, '-')



```

1004 FORMAT('1',/, '- ',10X,' ELECTRON - HELIUM + SCATTERING
1 PHASE SHIFT FOR',I3,' X ',I2,' HAMILTONIAN MATRIX.',/,
2 '- ',34X,'ALPHA =',F10.7,/, '0',24X,'TOTAL ENERGY, E =',
3 D24.16,/, '0',25X,'WAVE NUMBER, K =',D24.16,/, '0',15X,'
4 COULOMB PHASE SHIFT, ETA =',D24.16,/, '3',20X,'"NUCLEAR
5 CHARGE", Z =',F9.5)

1005 FORMAT(10I8)

1006 FORMAT('1',10X,'F = ',D10.3,/, '- ')

1007 FORMAT('0',5X,'ALPHA =',F9.6,4X,'K =',D24.16,5X,'
1 TANGENT(PHASE SHIFT) =',D24.16,/, '0',65X,'TAN(DELTA)/K
2 =',D24.16,/, '0',66X,'PHASE SHIFT =',D24.16)

1008 FORMAT      (8X,2I8,2I3,F10.3,5X,2F15.9)

1011 FORMAT('0',/, '- ',10X,'TRIPLET PHASE SHIFTS.')
1012 FORMAT('0',/, '- ',10X,'SINGLET PHASE SHIFTS.')
1013 FORMAT(10X,'TRACE OF (U*(-T))*H*(U*(-1)) =',D24.16)
1014 FORMAT('-',10X,'K(',I2,') =',D24.16,/, '- ')
1015 FORMAT(22X,'SUM OF EIGENVALUES =',D24.16,/)
1016 FORMAT(F11.7,F12.7)
1017 FORMAT('-',10X,I5,' CARDS PUNCHED FOR THIS JOB.')

1020 FORMAT('1',/, '- ',10X,' ELECTRON - HYDROGEN SCATTERING
1 PHASE SHIFT FOR',I3,' X ',I2,' HAMILTONIAN MATRIX.',/,
2 '- ',34X,'ALPHA =',F9.6,/, '0',24X,'TOTAL ENERGY, E =',
3 D23.16,/, '0',25X,'WAVE NUMBER, K =',D23.16)

1021 FORMAT(2I2,2I4,D8.3)

1100 FORMAT(F11.7,F12.7,3X,3D18.10)
1101 FORMAT(F11.7,F12.7,39X,D18.10)

3002 FORMAT('-',5X,'EIGENVALUES OF H FOR ALPHA = ',F12.7,/)
3004 FORMAT(4X,5D25.16)

3005 FORMAT('-',/,5X,'THE VALUES OF K FOR ALPHA =',F12.7,'
1 ARE:',/, '0')

      END

```



SUBROUTINE TBL1(MAX,A,B)

TBL1 GENERATES THE TABLE OF BOUND-BOUND INTEGRALS

IMPLICIT REAL\*8 (A-H,O-Z)

DIMENSION A(1),B(1)

THE INTEGRALS ARE STORED IN A ONE DIMENSIONAL ARRAY CORRESPONDING TO THE VARIOUS VALUES OF NU, LAMDA AND MU

MAX2 = MAX\*MAX

LIM = (MAX - 1)\*MAX2

INITIALIZE THE A AND B ARRAYS

DO 1 I=1,LIM

A(I) = .000

1 B(I) = .000

NMAX = MAX - 1

EVALUATE THE INTEGRALS FOR MU = 2

DO 2 NN=1,NMAX

DO 2 LL=2,MAX

IF((NN+LL.LT.5).OR.(NN+LL.GT.MAX+2)) GO TO 2

IN = NN + MAX\*(LL - 1) + 2\*MAX2

CALL SUM(NN,LL,AA)

A(IN) = AA

2 CONTINUE

USE THE RECURSION RELATIONS TO FIND THE INTEGRALS FOR MU = 1

DO 3 NN=2,MAX

DO 3 LL=2,MAX

IF((NN+LL.GT.MAX+3).OR.(NN+LL.LT.6)) GO TO 3

IN = NN + MAX\*(LL - 1) + MAX2

INP = IN + MAX2 - 1

A(IN) = A(INP)

IF((LL.LT.3).OR.(NN.LT.3).OR.(NN+LL.LT.6).OR.(LL.GE.1MAX).OR.(NN.GE.MAX)) GO TO 3

INP = IN + MAX\*(MAX + 1) - 2

B(IN) = A(INP)/.301

3 CONTINUE

MMAX = MAX - 1



NLMAX = MAX - 2

USE THE RECURSION RELATIONS TO FIND THE INTEGRALS FOR MU > 2

```
DO 5 MM=4,MMAX
DO 5 NN=2,NLMAX
DO 5 LL=2,NLMAX
IF((NN+LL.LT.5).OR.(NN+LL+MM.GT.MAX+5)) GO TO 5
IN = NN + MAX*(LL - 1) + (MM - 1)*MAX2
INN = IN - 2*(MAX2 - 1)
INL = IN - 2*MAX*(MAX - 1)
INN1 = IN - MAX*(2*MAX - 1) + 1
A(IN) = A(INN) + A(INL) - .2D1*B(INN1)
IF((MM.GT.MAX-3).OR.(NN+LL.LT.6).OR.(LL.LE.2).OR.(NN.
1LE.2).OR.(LL.GT.MAX-3).OR.(NN.GT.MAX-3)) GO TO 5
B(IN) = (B(INN) + B(INL) - .2D1*A(INN1))*DFLOAT(MM-3)/
1DFLOAT(MM+1)
5 CONTINUE
RETURN
END
```

SUBROUTINE SUM(NU,LMDA,CUT)

SUM EVALUATES A(NU,LAMDA,2) FOR GIVEN NU, LAMDA

```
IMPLICIT REAL*8 (A-H,O-Z)
EXTERNAL FACT
A = 0.0D0
NN = NU - 1
DO 10 I=1,LMDA
IN2 = LMDA - I
IN1 = NN + IN2
10 A = A + FACT(IN1)/(FACT(IN2)*(0.2D1**((IN1 + 1))))
LL = LMDA - 1
OUT = FACT(LL)*(FACT(NN) - A)
RETURN
END
```





DOUBLE PRECISION FUNCTION FACT(N)

FACT FORMS N FACTORIAL

IMPLICIT REAL\*8 (A-H,O-Z)

FACT = .1D1

IF(N.EQ.0) GO TO 20

DO 10 I=1,N

FI = I

10 FACT = FACT\*FI

20 RETURN

END



SUBROUTINE SPLIN1(X,Y,M,XINT,YINT)

SPLIN PROVIDES INTERPOLATED VALUE OF THE ORDINATE USING  
"CUBIC SPLINE FITTING"

USAGE:

FIRST CALL TO SUBROUTINE:

CALL SPLIN1(X,Y,M,XINT,YINT)

SUBSEQUENT CALLS USING THE SAME DATA

CALL SPLINN(X,Y,M,XINT,YINT)

DESCRIPTION OF PARAMETERS

X: MONOTONICALLY INCREASING ABSCISSA ARRAY

Y: ONE-FOR-ONE CORRESPONDING ORDINATE ARRAY

M: NUMBER OF X AND Y VALUES SUPPLIED < OR =  
300. (MODIFIED IN THE PRESENT CONTEXT TO  
NO MORE THAN FIVE)

XINT: VALUE OF ABSCISSA FOR WHICH CORRESPOND-  
ING ORDINATE IS TO BE INTERPOLATED (OR  
EXTRAPOLATED)

YINT: INTERPOLATED (OR EXTRAPOLATED) ORDINATE  
VALUE

MATHEMATICAL METHOD:

UPON FIRST ENTRY TO SPLIN, A CALL TO SPLICO IS  
MADE TO DETERMINE THE COEFFICIENTS TO BE USED IN  
PERFORMING THE INTERPOLATIONS. SEARCH FOR BRACKET-  
ING ABSCISSA VALUES IS ALWAYS MADE FROM THE REFER-  
ENCE LAST USED IN INTERPOLATING.

REFERENCE:

PENNINGTON, R.H., "INTRODUCTORY COMPUTER METHODS  
AND NUMERICAL ANALYSIS", MACMILLAN, NEW YORK, 1965

★ IMPLICIT REAL\*8 (A-H),REAL\*8 (O-Z)

DIMENSION X(M),Y(M),C(4,6)

CALL SPLICO(X,Y,M,C)

K=1

ENTRY SPLINN(X,Y,M,XINT,YINT)

3 IF(XINT-X(1)) 70,1,2

70 K=1

GO TO 7

1 YINT=Y(1)

RETURN

2 IF(XINT-X(K+1)) 6,4,5

4 YINT=Y(K+1)

RETURN

5 K=K+1

IF(M-K) 71,71,3

71 K=M-1

GO TO 7

6 IF(XINT-X(K)) 13,12,11

12 YINT=Y(K)

RETURN



```

13 K=K-1
   GO TO 6
7 PRINT 101,XINT
101 FORMAT(8H0XINT = E18.9,32H, OUT OF RANGE FOR
1 INTERPOLATION)
11 YINT=(X(K+1)-XINT)*(C(1,K)*(X(K+1)-XINT)**2+C(3,K))
   YINT=YINT+(XINT-X(K))*(C(2,K)*(XINT-X(K))**2+C(4,K))
   RETURN
END

```

```

SUBROUTINE SPLICO(X,Y,M,C)
  IMPLICIT REAL*8 (A-H),REAL*8 (O-Z)
  DIMENSION X(M),Y(M),C(4,6),D(6),P(6),E(6),A(6,3),B(6),
1 Z(6)
  MM=M-1
  DO 2 K=1,MM
    D(K)=X(K+1)-X(K)
    P(K)=D(K)/6.
2 E(K)=(Y(K+1)-Y(K))/D(K)
  DO 3 K=2,MM
3 B(K)=E(K)-E(K-1)
  A(1,2)=-1.-D(1)/D(2)
  A(1,3)=D(1)/D(2)
  A(2,3)=P(2)-P(1)*A(1,3)
  A(2,2)=2.*(P(1)+P(2))-P(1)*A(1,2)
  A(2,3)=A(2,3)/A(2,2)
  B(2)=B(2)/A(2,2)
  DO 4 K=3,MM
    A(K,2)=2.*(P(K-1)+P(K))-P(K-1)*A(K-1,3)
    B(K)=B(K)-P(K-1)*B(K-1)
    A(K,3)=P(K)/A(K,2)
4 B(K)=B(K)/A(K,2)
  Q=D(M-2)/D(M-1)
  A(M,1)=1.+Q+A(M-2,3)
  A(M,2)=-Q-A(M,1)*A(M-1,3)
  B(M)=B(M-2)-A(M,1)*B(M-1)

```



```

Z(M)=B(M)/A(M,2)
MN=M-2
DO 6 I=1,MN
K=M-I
6 Z(K)=B(K)-A(K,3)*Z(K+1)
Z(1)=-A(1,2)*Z(2)-A(1,3)*Z(3)
DO 7 K=1,MM
Q=1./(6.*D(K))
C(1,K)=Z(K)*Q
C(2,K)=Z(K+1)*Q
C(3,K)=Y(K)/D(K)-Z(K)*P(K)
7 C(4,K)=Y(K+1)/D(K)-Z(K+1)*P(K)
RETURN
END

```





SUBROUTINE ELEM(HH,SS,A,B,MAX)

ELEM GENERATES THE MATRIX ELEMENTS  $\langle \text{CHI}(I) | H | \text{CHI}(J) \rangle$  AND  $\langle \text{CHI}(I) | \text{CHI}(J) \rangle$  FOR H AND S, RESPECTIVELY

IMPLICIT REAL\*8 (A-H,O-Z)

INTEGER PWR

COMMON/TRM/ALFA,ETA

COMMON/ATNO/Z

COMMON/INDEX/NI,NJ,LI,LJ,MI,MJ,IS

DIMENSION A(1),B(1),NU(52),MU(52),LMDA(52),COEF(52)

NIJ = NI + NJ

LIJ = LI + LJ

NLIJ = NI + LJ

LNIJ = LI + NJ

MIJ = MI + MJ

FN1 = DFLOAT(NJ + 1)

FL1 = DFLOAT(LJ + 1)

FN = DFLOAT(NJ)

FL = DFLOAT(LJ)

FM = DFLOAT(MJ)

MAX2 = MAX\*MAX

SET THE VALUES OF NJ, LAMDA, MU AND THE COEFFICIENTS FOR EACH OF THE 52 TERMS OF H(I,J) AND THE 4 TERMS OF S(I,J)

NU( 1) = NIJ + 2

NU( 3) = NU(1)

NU( 4) = NU(1)

NU( 6) = NU(1)

NU( 8) = NU(1)

NU( 9) = NU(1)

NU(37) = NU(1)

LMDA(10) = NU( 1)

LMDA(11) = NU( 1)

LMDA(14) = NU( 1)

LMDA(15) = NU( 1)

LMDA(16) = NU( 1)

LMDA(18) = NU( 1)



```

LMDA(42) = NU( 1)
NU( 2) = NIJ + 1
LMDA(12) = NU( 2)
NU(39) = NU(2)
LMDA(44) = NU( 2)
NU( 5) = NIJ + 3
NU(38) = NU(5)
NU(40) = NU(5)
LMDA(13) = NU( 5)
LMDA(41) = NU(5)
LMDA(43) = NU( 5)
NU( 7) = NIJ
LMDA(17) = NU( 7)
NU(10) = LIJ + 2
NU(12) = NU(10)
NU(13) = NU(10)
NU(15) = NU(10)
NU(17) = NU(10)
NU(18) = NU(10)
NU(41) = NU(10)
LMDA( 1) = NU(10)
LMDA( 2) = NU(10)
LMDA( 5) = NU(10)
LMDA( 6) = NU(10)
LMDA( 7) = NU(10)
LMDA( 9) = NU(10)
LMDA(38) = NU(10)
NU(11) = LIJ + 1
LMDA( 3) = NU(11)
NU(43) = NU(11)
LMDA(40) = NU(11)
NU(14) = LIJ + 3
LMDA( 4) = NU(14)
NU(42) = NU(14)
NU(44) = NU(14)
LMDA(37) = NU(14)

```



```

LMDA(39) = NU(14)
NU(16) = LIJ
LMDA( 8) = NU(16)
NU(19) = NLIJ + 2
NU(21) = NU(19)
NU(22) = NU(19)
NU(24) = NU(19)
NU(26) = NU(19)
NU(27) = NU(19)
NU(45) = NU(19)
LMDA(28) = NU(19)
LMDA(29) = NU(19)
LMDA(32) = NU(19)
LMDA(33) = NU(19)
LMDA(34) = NU(19)
LMDA(36) = NU(19)
LMDA(50) = NU(19)
NU(20) = NLIJ + 1
NU(47) = NU(20)
LMDA(30) = NU(20)
LMDA(52) = NU(20)
NU(23) = NLIJ + 3
NU(46) = NU(23)
NU(48) = NU(23)
LMDA(31) = NU(23)
LMDA(49) = NU(23)
LMDA(51) = NU(23)
NU(25) = NLIJ
LMDA(35) = NU(25)
NU(28) = LNIJ + 2
NU(30) = NU(28)
NU(31) = NU(28)
NU(33) = NU(28)
NU(35) = NU(28)
NU(36) = NU(28)
NU(49) = NU(28)

```



```

LMDA(19) = NU(28)
LMDA(20) = NU(28)
LMDA(23) = NU(28)
LMDA(24) = NU(28)
LMDA(25) = NU(28)
LMDA(27) = NU(28)
LMDA(46) = NU(28)
NU(29) = LNIJ + 1
NU(51) = NU(29)
LMDA(21) = NU(29)
LMDA(48) = NU(29)
NU(32) = LNIJ + 3
LMDA(22) = NU(32)
NU(50) = NU(32)
NU(52) = NU(32)
LMDA(45) = NU(32)
LMDA(47) = NU(32)
NU(34) = LNIJ
LMDA(26) = NU(34)
MU( 1) = MIJ + 2
MU( 2) = MU(1)
MU( 3) = MU(1)
MU( 7) = MU(1)
MU( 8) = MU(1)
MU(10) = MU(1)
MU(11) = MU(1)
MU(12) = MU(1)
MU(16) = MU(1)
MU(17) = MU(1)
MU(19) = MU(1)
MU(20) = MU(1)
MU(21) = MU(1)
MU(25) = MU(1)
MU(26) = MU(1)
MU(28) = MU(1)
MU(29) = MU(1)

```





```

MU(30) = MU(1)
MU(34) = MU(1)
MU(35) = MU(1)
MU( 4) = MIJ
MU( 5) = MU(4)
MU( 6) = MU(4)
MU(13) = MU(4)
MU(14) = MU(4)
MU(15) = MU(4)
MU(22) = MU(4)
MU(23) = MU(4)
MU(24) = MU(4)
MU(31) = MU(4)
MU(32) = MU(4)
MU(33) = MU(4)
MU(37) = MU(4)
MU(38) = MU(4)
MU(39) = MU(4)
MU(40) = MU(4)
MU(41) = MU(4)
MU(42) = MU(4)
MU(43) = MU(4)
MU(44) = MU(4)
MU(45) = MU(4)
MU(46) = MU(4)
MU(47) = MU(4)
MU(48) = MU(4)
MU(49) = MU(4)
MU(50) = MU(4)
MU(51) = MU(4)
MU(52) = MU(4)
MU( 9) = MIJ + 1
MU(18) = MU(9)
MU(27) = MU(9)
MU(36) = MU(9)
COEF( 1) = -0.25D0*ALFA*ALFA

```



```

COEF(10) = COEF(1)
COEF(19) = COEF(1)
COEF(28) = COEF(1)
COEF( 2) = 0.5D0*ALFA*FN1 - Z
COEF(12) = COEF(2)
COEF(21) = COEF(2)
COEF(29) = COEF(2)
COEF( 3) = 0.5D0*ALFA*FL1 - Z
COEF(11) = COEF(3)
COEF(20) = COEF(3)
COEF(30) = COEF(3)
COEF( 4) = 0.5D0*ALFA*FM
COEF( 5) = COEF(4)
COEF(13) = COEF(4)
COEF(14) = COEF(4)
COEF(22) = COEF(4)
COEF(23) = COEF(4)
COEF(31) = COEF(4)
COEF(32) = COEF(4)
COEF(37) = -COEF(4)
COEF(38) = -COEF(4)
COEF(41) = -COEF(4)
COEF(42) = -COEF(4)
COEF(45) = -COEF(4)
COEF(46) = -COEF(4)
COEF(49) = -COEF(4)
COEF(50) = -COEF(4)
COEF( 6) = -FM*(FM + FN + FL1)
COEF(15) = COEF(6)
COEF(24) = COEF(6)
COEF(33) = COEF(6)
COEF( 7) = -0.5D0*FN*FN1
COEF(17) = COEF(7)
COEF(26) = COEF(7)
COEF(34) = COEF(7)
COEF( 8) = -0.5D0*FL*FL1

```



```

COEF(16) = COEF(8)
COEF(25) = COEF(8)
COEF(35) = COEF(8)
COEF( 9) = 0.1D1
COEF(18) = COEF(9)
COEF(27) = COEF(9)
COEF(36) = COEF(9)
COEF(39) = FM*FN
COEF(44) = COEF(39)
COEF(48) = COEF(39)
COEF(51) = COEF(39)
COEF(40) = FM*FL
COEF(43) = COEF(40)
COEF(47) = COEF(40)
COEF(52) = COEF(40)
MAX2 = MAX*MAX
HH     = 0.0D0
IF(IS.EQ.0) GO TO 10

```

FOR TRIPLET SCATTERING THE SIGNS OF THE LAST 26 TERMS IN  
H(I,J) MUST BE CHANGED

```

DO 1 I=19,36
1 COEF(I) = -COEF(I)
DO 2 I=45,52
2 COEF(I) = -COEF(I)

```

THE VALUES OF NU, LAMDA AND MU FOUND ABOVE MUST BE CONVERTED  
TO A SINGLE INDEX CORRESPONDING TO THE STORAGE MODE OF THE  
INTEGRALS

```

10 DO 6 K=1,36
    IN = NU(K) + 1 + MAX*LMDA(K) + MU(K)*MAX2
    PWR = NU(K) + LMDA(K) + MU(K)
6  HH     = HH     + COEF(K)*A(IN)/ALFA**PWR
    DO 7 K=37,52
    IN = NU(K) + 1 + MAX*LMDA(K) + MU(K)*MAX2
    PWR = NU(K) + LMDA(K) + MU(K)
7  HH     = HH     + COEF(K)*B(IN)/ALFA**PWR

```

AFTER FORMATION OF H(I,J) THE SAME PROCESS MUST BE REPEATED  
FOR S(I,J)



```

SS = 0.000
DO 9 K=1,10,9
  IN = NU(K) + 1 + MAX*LMDA(K) + MU(K)*MAX2
  PWR = NU(K) + LMDA(K) + MU(K)
9  SS = SS + A(IN)/ALFA**PWR
  IF (IS.EQ.0) GO TO 11
  DO 13 K=19,28,9
    IN = NU(K) + 1 + MAX*LMDA(K) + MU(K)*MAX2
    PWR = NU(K) + LMDA(K) + MU(K)
13  SS = SS - A(IN)/ALFA**PWR
    GO TO 12
11 DO 8 K=19,28,9
    IN = NU(K) + 1 + MAX*LMDA(K) + MU(K)*MAX2
    PWR = NU(K) + LMDA(K) + MU(K)
8   SS = SS + A(IN)/ALFA**PWR
12 RETURN
END

```





SUBROUTINE SCL(S,N,F)

SCL FINDS THE ORDER OF MAGNITUDE OF THE LARGEST (ABSOLUTE  
VALUE) ELEMENT IN A GIVEN MATRIX

IMPLICIT REAL\*8 (A-H,O-Z)

DIMENSION S(1)

TOP = DABS(S(1))

DO 100 I=1,N

T = DABS(S(I))

IF(T.GT.TOP) TOP = T

100 CONTINUE

FF, = DLOG10(TOP)

IPWR = IDINT(FF)

F = 0.1D2\*\*(-IPWR)

RETURN

END

SUBROUTINE SMPY(A,C,N)

SMPY MULTIPLIES A MATRIX BY A SCALAR, RETURNING THE SCALED  
MATRIX IN THE SAME LOCATION AS THE ORIGINAL MATRIX

IMPLICIT REAL\*8 (A-H,O-Z)

DIMENSION A(1)

DO 1 I=1,N

1 A(I) = A(I)\*C

RETURN

END



SUBROUTINE INVERT(TS,H,S,C,N,ISIZE)

INVERT TAKES THE SYMMETRIC, POSITIVE DEFINITE MATRIX S (STORED IN THE COMPRESSED MODE IN TS) AND, USING DSINV, FACTORS IT INTO ITS UPPER TRIANGULAR FACTOR AND INVERTS THIS FACTOR. THEN USING THIS RESULT AS A FIRST APPROXIMATION THE INVERSE IS IMPROVED BY AN ITERATION METHOD

IMPLICIT REAL\*8 (A-H,O-Z)

REAL\*4 EPS

DIMENSION TS(1),H(1),S(1),C(1)

KIT = 0

EPS = 0.1E-7

CALL DSINV(TS,C,N,EPS,IER)

IF(IER.EQ.-1) GO TO 16

ISIG = 1

U\*\*(-1) (IN TS) AND U (IN C) ARE MULTIPLIED TO FORM A TRIAL IDENTITY WHICH IS CHECKED FOR OFF-DIAGONAL ELEMENTS WHICH MAY BE > 10\*\*(-20), AND STORED IN THE LOWER TRIANGLE OF H

DO 3 K=2,N

KK = K - 1

KM = K\*(K - 1)/2

DO 2 I=1,KK

IK = K + N\*(I - 1)

CC = 0.000

DO 1 J=I,K

IJ = J\*(J - 1)/2 + I

JK = KM + J

1 CC = CC + C(IJ)\*TS(JK)

IF(DABS(CC).GT.0.1D-20) ISIG = 0

2 H(IK) = -CC

3 CONTINUE

IF THE INVERSE IS ALREADY GOOD ENOUGH NO IMPROVEMENT IS NEEDED AND RETURN TO THE MAIN PROGRAM CAN BE MADE

IF(ISIG.EQ.1) GO TO 15

14 KIT = KIT + 1

THE CORRECTION TERM IS FORMED BY MULTIPLYING U\*\*(-1) AND THE TRIAL INVERSE

DO 6 K=2,N



```

KK = K - 1
KM = K*(K - 1)/2
DO 5 I=1, KK
IN = N*(I - 1)
IK = K + IN
II = I + 1
CC = 0.000
DO 4 J=II, K
IJ = J + IN
JK = KM + J
4 CC = CC + H(IJ)*TS(JK)
5 S(IK) = CC
6 CONTINUE

```

THE IMPROVED INVERSE IS FORMED BY ADDING THE CORRECTION TERM  
TO  $U^{**}(-1)$

```

DO 8 K=2, N
KK = K - 1
KM = K*(K - 1)/2
DO 7 I=1, KK
IK = KM + I
KI = K + N*(I - 1)
7 TS(IK) = TS(IK) + S(KI)
8 CONTINUE
ISIG = 1

```

THE NEW TRIAL INVERSE IS FORMED AND TESTED FOR ANY ELEMENTS  
>  $10^{**}(-20)$ . THIS VALUE IS PUT IN THE LOWER TRIANGLE OF S

```

DO 11 K=2, N
KK = K - 1
DO 10 I=1, KK
IN = N*(I - 1)
IK = K + IN
CC = 0.000
II = I + 1
IF(II.GT.KK) GO TO 10
DO 9 J=II, KK
IJ = J + IN

```



```

      JK = K + N*(J - 1)
9  CC = CC + H(IJ)*H(JK)
      IF(DABS(CC).GT.0.1D-20) ISIG = 0
10 S(IK) = CC
11 CONTINUE
      IF(ISIG.EQ.1) GO TO 15

IF THE INVERSE IS STILL NOT GOOD ENOUGH THE NEW TRIAL IN-
VERSE IS PUT IN H AND THE PROCESS IS REPEATED
      DO 13 K=2,N
      KK = K - 1
      DO 12 I=1,KK
      IK = K + N*(I - 1)
12 H(IK) = S(IK)
13 CONTINUE
      GO TO 14
15 WRITE(6,1001) KIT
      RETURN
16 WRITE(6,1000)
      STOP
1000 FORMAT(10X,'STOP. IER =-1, AND S CANNOT BE FACTORED.')
1001 FORMAT('-',10X,'INVERSE FOUND AFTER',I2,'ITERATIONS.')
      END

```

#### SUBROUTINE DSINV(A,C,N,EPS,IER)

DSINV INVERTS A GIVEN SYMMETRIC POSITIVE DEFINITE MATRIX  
(MODIFIED IN THE PRESENT CONTEXT TO PROVIDE ONLY THE INVERSE  
OF THE UPPER TRIANGULAR FACTOR OF A)

DESCRIPTION OF PARAMETERS:

A: DOUBLE PRECISION UPPER TRIANGULAR PART OF  
GIVEN SYMMETRIC POSITIVE DEFINITE N BY N  
COEFFICIENT MATRIX. ON RETURN A CONTAINS  
THE RESULTANT UPPER TRIANGULAR MATRIX IN  
DOUBLE PRECISION  
C: MATRIX IN WHICH THE UPPER TRIANGULAR FACTOR  
OF A IS STORED FOR LATER USE IN THE CALLING  
PROGRAM  
N: THE NUMBER OF ROWS (COLUMNS) IN THE GIVEN  
MATRIX  
EPS: SINGLE PRECISION INPUT CONSTANT WHICH IS  
USED AS A RELATIVE TOLERANCE FOR TEST ON  
LOSS OF SIGNIFICANCE  
IER: RESULTING ERROR PARAMETER CODED AS FOLLOWS  
IER=0 NO ERROR  
IER=-1 NO RESULT BECAUSE OF WRONG INPUT





PARAMETER N OR BECAUSE SOME RAD-  
 ICAND IS NON-POSITIVE (MATRIX A  
 IS NOT POSITIVE DEFINITE, POS-  
 SIBLY DUE TO LOSS OF SIGNIFI-  
 CANCE)  
 WARNING WHICH INDICATES LOSS OF  
 SIGNIFICANCE. THE RADICAND  
 FORMED AT FACTORIZATION STEP K+1  
 WAS STILL POSITIVE BUT NO LONGER  
 > |EPS\*A(K+1,K+1)|

IER=K

DOUBLE PRECISION A,DIN,WORK,C

DIMENSION A(1),C(1)

FIND THE UPPER TRIANGULAR FACTOR OF A

CALL DMFSD(A,N,EPS,IER)

IF(IER) 9,1,1

INVERT UPPER TRIANGULAR MATRIX T  
 PREPARE INVERSION LOOP

1 IPIV=N\*(N+1)/2

IND=IPIV

SAVE T BY DUPLICATING IT IN C

DO 7 I=1,IPIV

7 C(I) = A(I)

INITIALIZE INVERSION-LOOP

DO 6 I=1,N

DIN=1.0/A(IPIV)

A(IPIV)=DIN

MIN=N

KEND=I-1

LANF=N-KEND

IF(KEND) 5,5,2

2 J=IND

DO 4 K=1,KEND

INITIALIZE ROW-LOOP

WORK=0.0

MIN=MIN-1

LHOR=IPIV

LVER=J

START INNER LOOP



```

      DO 3 L=LANF,MIN
      LVER=LVER+1
      LHOR=LHOR+L
3    WORK=WORK+A(LVER)*A(LHOR)
      A(J)=-WORK/DIN
4    J=J-MIN
5    IPIV=IPIV-MIN
6    IND=IND-1
9    RETURN
      END

```

SUBROUTINE DMFSD(A,N,EPS,IER)

DMFSD FACTORS A GIVEN SYMMETRIC, POSITIVE DEFINITE MATRIX INTO ITS UPPER AND LOWER TRIANGULAR FACTORS (WHICH ARE THE TRANSPOSE OF EACH OTHER). THE SOLUTION IS DONE USING THE SQUARE ROOT METHOD OF CHOLESKY.

DIMENSION A(1)

DOUBLE PRECISION DPIV,DSUM,A

TEST ON WRONG INPUT PARAMETER N

IF(N-1) 12,1,1

1 IER=0

INITIALIZE DIAGONAL LOOP

KPIV=0

DO 11 K=1,N

KPIV=KPIV+K

IND=KPIV

LEND=K-1

CALCULATE TOLERANCE

TOL=ABS(EPS\*SVGL(A(KPIV)))

START FACTORIZATION LOOP OVER K-TH ROW

DO 11 I=K,N

DSUM=0.DO

IF(LEND) 2,4,2



START INNER LOOP

2 DO 3 L=1,LEND

LANF=KPIV-L

LIND=IND-L

3 DSUM=DSUM+A(LANF)\*A(LIND)

TRANSFORM ELEMENT A(IND)

4 DSUM=A(IND)-DSUM

IF(I-K) 10,5,10

TEST FOR NEGATIVE PIVOT ELEMENT AND FOR LOSS OF SIGNIFICANCE

5 IF(SNGL(DSUM)-TOL) 6,6,9

6 IF(DSUM) 12,12,7

7 IF(IER) 8,8,9

8 IER=K-1

COMPUTE PIVOT ELEMENT

9 DPIV=DSQRT(DSJM)

A(KPIV)=DPIV

DPIV=1.00/DPIV

GO TO 11

CALCULATE TERMS IN ROW

10 A(IND)=DSUM\*DPIV

11 IND=IND+1

RETURN

12 IER=-1

RETURN

END



SUBROUTINE TMPRD(H,U,C,N,F)

TMPRD FORMS THE MATRIX PRODUCT  $U^{**}(-T)*H*U^{**}(-1)$  AND THEN MULTIPLIES IT BY THE SAME FACTOR AS WAS USED TO SCALE S

```
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION H(1),U(1),C(1)
LIM = N*(N + 1)/2
DO 3 L=1,N
DO 3 K=L,N
LK = K*(K - 1)/2 + L
UHU = 0.000
DO 2 I=1,L
HU = 0.000
IL = L*(L - 1)/2 + I
DO 1 J=1,K
IJ = J*(J - 1)/2 + I
IF(I.GT.J) IJ = I*(I - 1)/2 + J
JK = K*(K - 1)/2 + J
1 HU = HU + H(IJ)*U(JK)
2 UHU = UHU + U(IL)*HU
3 C(LK) = UHU
DO 4 I=1,LIM
4 H(I) = C(I)*F
RETURN
END
```





# SUBROUTINE DJACVT (A,N,NOYES,EIVU,EIVR,NDIM)

DJACVT CALCULATES IN DOUBLE PRECISION ALL THE EIGENVALUES OF A REAL, SYMMETRIC MATRIX BY USE OF THE JACOBI VARIABLE THRESHOLD METHOD. CORRESPONDING ORTHOGONAL EIGENVECTORS ARE ALSO CALCULATED, IF DESIRED. ORIGINALLY PROGRAMMED BY W. POOLE, COMPUTER CENTER, U. C., BERKELEY.

## DESCRIPTION OF PARAMETERS

A: THE REAL\*8 SYMMETRIC (SQUARE) MATRIX WHOSE EIGENVALUES AND EIGENVECTORS ARE SOUGHT. ROW DIMENSION MUST BE NDIM.  
 N: ORDER OF A,  $0 < N \leq NDIM \leq 161$   
 NOYES: INDICATOR SUPPLIED BY USER.  
       NOYES=0 EIGENVECTORS ARE NOT WANTED  
       NOYES=1 EIGENVECTORS ARE WANTED  
 EIVU: THE EIGENVALUES ARE RETURNED IN THIS VECTOR, WHICH MUST BE DIMENSIONED TO AT LEAST N IN CALLING PROGRAM. THEY ARE IN NO PARTICULAR ORDER.  
 EIVR: THE EIGENVECTORS (IF REQUESTED) ARE RETURNED AS THE COLUMNS OF THIS MATRIX, THE ROW DIMENSION OF WHICH MUST BE NDIM IN THE CALLING PROGRAM. THE COLUMN DIMENSION MUST BE AT LEAST N IN THE CALLING PROGRAM. THE VECTOR EIVR(I,J),  $I=1,N$  CORRESPONDS TO THE EIGENVALUE EIVU(J). IF EIGENVECTORS ARE NOT REQUESTED, AN UNDIMENSIONED VARIABLE SHOULD BE PUT IN THE POSITION OF EIVR IN THE CALL STATEMENT.  
 NDIM: THE ROW DIMENSION (FIRST DIMENSION) OF A AND EIVR IN THE DIMENSION STATEMENT OF THE CALLING PROGRAM.  $NDIM \leq 161$

## REMARKS

- 1) MATRIX A IS DESTROYED DURING CALCULATION.
- 2) ALL EIGENVALUES ARE CALCULATED EACH TIME DJACVT IS CALLED
- 3) VARIOUS DIAGNOSTIC MESSAGES MAY BE SENT TO STANDARD OUTPUT MEDIUM BY DJACVT. THESE INDICATE IMPROPER ARGUMENTS AND ARE GENERALLY SELF-EXPLANATORY.
- 4) LIMIT OF 160 FOR N (AND NDIM) COULD BE RAISED BY CHANGING STATEMENT 21

## REFERENCES

VON NEUMAN, J., AND GOLDSTEIN, "THE JACOBI METHOD FOR REAL SYMMETRIC MATRICES", JOURNAL OF ACM, 1, 1959  
 WILKINSON, J. H., "THE ALGEBRAIC EIGENVALUE PROBLEM OXFORD UNIVERSITY PRESS, 1965, P. 277 FF.

IMPLICIT REAL\*8(A-H,O-Z)

DIMENSION A(NDIM,NDIM),EIVU(NDIM),EIVR(NDIM,NDIM)

IF(N-1)20,23,21

20 PRINT 22,N

22 FORMAT(' N= ',I3,' IS TOO SMALL. LIMIT IS 1. RETURN  
 1 TO CALLING ROUTINE FROM DJACVT.')

RETURN

23 PRINT 24, A(1,1)

24 FORMAT (24H IN DJACVT , MATRIX A = ,E14.6)

RETURN



```

21 IF(N-160)1,1,3
3 PRINT 2,N
2 FORMAT(' N= ',I3,' IS TOO LARGE. LIMIT IS 160. RETURN
1 TO CALLING ROUTINE FROM DJACVT.')
```

RETURN

```

1 IF(NOYES)99,102,99
99 CONTINUE
DO 101 J=1,N
DO 100 I=1,N
100 EIVR(I,J)=0.0
101 EIVR(J,J)=1.0
102 ATOP=0.
DO 112 J=1,N
DO 111 I=1,J
IF(A(I,J)-A(J,I))90,103,90
90 PRINT 106,N,N
106 FORMAT(14H IN DJACVT (A(,I3,1H,,I3,3H)),)
PRINT 108,I,J,J,I
108 FORMAT(' A(,I3,',',I3,') AND A(,I3,',',I3,') WERE
1 UNEQUAL. THEY WERE REPLACED BY THEIR MEAN IN DJACVT')
A(I,J)=.5*(A(I,J)+A(J,I))
A(J,I)=A(I,J)
103 CONTINUE
IF(ATOP-DABS(A(I,J)))104,111,111
104 ATOP=DABS(A(I,J))
111 CONTINUE
112 EIVU(J)=A(J,J)
IF(ATOP)109,109,113
109 PRINT 110
110 FORMAT(26H IN DJACVT, MATRIX A = 0 )
RETURN
113 AVGF=DFLOAT(N*(N-1))*0.55
D=0.0
DO 114 JJ=2,N
DO 114 II=2,JJ
S=A(II-1,JJ)/ATOP
114 D=S*S+D
```



```

DSTOP=(1.D-06)*D
THRSH =DSQRT (D/AVGF)*ATOP
115 IFLAG=0
DO 130 JCOL=2,N
JCOL1=JCOL-1
DO 130 IROW=1,JCOL1
AIJ=A(IROW,JCOL)
IF(DABS(AIJ)-THRSH)130,130,117
117 AII=A(IROW,IROW)
AJJ=A(JCOL,JCOL)
S=AJJ-AII
IF(DABS(AIJ)-1.D-09*DABS(S))130,130,118
118 IFLAG=1
IF(1.D-10*DABS(AIJ)-DABS(S))116,119,119
119 S=.7071067811865475
C=S
GO TO 120
116 T=AIJ/S
S=0.25/DSQRT(0.25+T*T)
C=DSQRT(0.5+S)
S=2.*T*S/C
120 DO 121 I=1,IROW
T=A(I,IROW)
U=A(I,JCOL)
A(I,IROW)=C*T-S*U
121 A(I,JCOL)=S*T+C*U
I2=IROW+2
IF(I2-JCOL)127,127,123
127 CONTINUE
DO 122 I=I2,JCOL
T=A(I-1,JCOL)
U=A(IROW,I-1)
A(I-1,JCOL)=S*U+C*T
122 A(IROW,I-1)=C*U-S*T
123 A(JCOL,JCOL)=S*AIJ+C*AJJ
A(IROW,IROW)=C*A(IROW,IROW)-S*(C*AIJ-S*AJJ)

```



```

      DO 124 J=JCOL,N
      T=A(IROW,J)
      U=A(JCOL,J)
      A(IROW,J)=C*T-S*U
124  A(JCOL,J)=S*T+C*U
      IF(NOYES)131,126,131
131  CONTINUE
      DO 125 I=1,N
      T=EIVR(I,IROW)
      EIVR(I,IROW)=C*T-EIVR(I,JCOL)*S
125  EIVR(I,JCOL)=S*T+EIVR(I,JCOL)*C
126  CONTINUE
      S=AIJ/ATOP
      D=D-S*S
      IF(D-DSTOP)1260,129,129
1260 D=0.
      DO 128 JJ=2,N
      DO 128 II=2,JJ
      S=A(II-1,JJ)/ATOP
128  D=S*S+D
      DSTOP=(1.D-06)*D
129  THRSH=DSQRT(D/AVGF)*ATOP
130  CONTINUE
      IF(IFLAG)115,134,115
134  T=A(1,1)
      A(1,1)=EIVU(1)
      EIVU(1)=T
      DO 132 J=2,N
      T=A(J,J)
      A(J,J)=EIVU(J)
      EIVU(J)=T
      DO 132 I=2,J
132  A(I-1,J)=A(J,I-1)
133  RETURN
      END

```





SUBROUTINE MPRD(A,B,C,N)

MPRD FORMS THE MATRIX PRODUCT  $A*B$ . THE RESULT IS RETURNED  
IN B. C IS USED FOR TEMPORARY STORAGE.

```
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION A(1),B(1),C(1)
DO 2 I=1,N
DO 2 K=1,N
IK = N*(K-1) + I
CC = 0.0D0
DO 1 J=1,N
IJ = N*(J-1) + I
JK = N*(K-1) + J
1 CC = CC + A(IJ)*B(JK)
2 C(IK) = CC
LIM = N*N
DO 3 I=1,LIM
3 B(I) = C(I)
RETURN
END
```



SUBROUTINE INT256(FCT,F)

INT256 IS A 256-POINT GAUSS-LEGENDRE QUADRATURE USING AN EXTERNALLY DEFINED FUNCTION. THE SAMPLE POINTS, WEIGHT VALUES AND INTEGRATION SEGMENTS ARE READ INTO THE CALLING PROGRAM FROM AN EXTERNAL SOURCE

IMPLICIT REAL\*8 (A-H,O-Z)

COMMON/L256/X(128),A(128)

COMMON/CD/DPC(15),DMC(15)

F = 0.000

DO 100 I=1,128

ZZZ = 0.000

XX = X(I)

AA = A(I)

TO MINIMIZE COMPUTATION TIME THE INTEGRAND IS COMPUTED AT THE SAME RELATIVE POINT IN ALL 15 INTEGRATION INTERVALS FIRST AND THEN THE SUM OF THESE VALUES IS MULTIPLIED BY THE WEIGHT FACTOR FOR THAT POINT

DO 10 J=1,15

THE DPC AND DMC ARE, RESPECTIVELY,  $(D+C)/2$  AND  $(D-C)/2$ , WHERE D AND C ARE THE UPPER AND LOWER INTEGRATION LIMITS

DP = DPC(J)

DM = DMC(J)

CHANGE THE VARIABLE TO CONFORM TO THE -1,+1 INTERVAL REQUIRED IN GAUSS-LEGENDRE QUADRATURE

P = XX\*DM

ZP = DP + P

ZM = DP - P

10 ZZZ = ZZZ + DM\*(FCT(ZP) + FCT(ZM))

100 F = F + ZZZ\*AA

RETURN

END

DOUBLE PRECISION FUNCTION CGARG(Z)

CGARG EVALUATES THE INTEGRAND AT THE DESIGNATED POINT FOR THE GAMMA FUNCTION INTEGRATIONS

IMPLICIT REAL\*8 (A-H,O-Z)



```
COMMON/CONST/PH1,PH2,FR1,FR2,SCL,TWOPI,FCT2,FCT1,A  
ARG = A*DLOG(Z)  
CGARG = (Z**3)*DEXP(-Z)*(FCT2*DSIN(ARG) + FCT1*DCOS(ARG))  
RETURN  
END
```



SUBROUTINE TBL2(IMAX,MAXI,AS,AC,BS,BC)

TBL2 TABULATES THE REQUIRED BOUND-FREE INTEGRALS

IMPLICIT REAL\*8 (A-H,O-Z)

COMMON/CONST/PH1,PH2,FR1,FR2,ASCL,PI,CA,CT,AAA

COMMON/WAVP/WAV

COMMON/TRM/ALFA,ETA

COMMON/ATNO/Z

COMMON/RHO/N

DIMENSION AC(1),AS(1),BC(1),BS(1)

DIMENSION A1(144),A2(144)

DIMENSION S1(13),C2(13),SS(11),CC(11)

DIMENSION X0(500)

ALFA2 = ALFA + Z

CALCULATE THE FREQUENCY AND PHASE FACTORS IN THE SINUSOIDAL  
TERMS

FR1 = WAV/ALFA2

PH1 = AAA\*DLOG(.2D1\*FR1) + ETA

FR2 = .2D1\*WAV/ALFA

PH2 = AAA\*DLOG(.2D1\*FR2) + ETA

ASCL = 0.5D0\*ALFA/ALFA2

WRITE(6,3000) PH1,FR1,PH2,FR2,ASCL

IF Z=1 THE NUMERICAL INTEGRATIONS NEED NOT BE DONE

IF(AAA.EQ.0.0D0) GO TO 104

FIND THE ZEROES OF THE INTEGRAND FOR I1

CALL ZERO(1,L,X0,IQ)

EVALUATE THE I1 INTEGRALS

DO 100 I=1,IMAX

N = I - 2

CALL CSINT(1,L,IQ,X0,ZZ,ASCL)

100 S1(I) = ZZ

FIND THE ZEROES OF THE INTEGRAND FOR IS

CALL ZERO(2,L,X0,IQ)





EVALUATE THE IS INTEGRALS

DO 101 I=1,MAXI

N = I - 2

CALL CSINT(2,L,IQ,X0,ZZ,0.1D1)

101 SS(I) = ZZ

FIND THE ZEROES OF THE INTEGRAND FOR I3

CALL ZERO(3,L,X0,IQ)

EVALUATE THE I3 INTEGRALS

DO 102 I=1,IMAX

N = I - 2

CALL CSINT(3,L,IQ,X0,ZZ,ASCL)

102 C2(I) = ZZ

FIND THE ZEROES OF THE INTEGRAND FOR IC

CALL ZERO(4,L,X0,IQ)

EVALUATE THE IC INTEGRALS

DO 103 I=1,MAXI

N = I - 2

CALL CSINT(4,L,IQ,X0,ZZ,0.1D1)

103 CC(I) = ZZ

GO TO 105

FOR Z=1 EVALUATE THE REQUIRED INTEGRALS EXACTLY

104 CALL HINT(S1,C2,SS,CC,IMAX,MAXI)

105 WRITE(6,2001)

WRITE(6,2000)(J,S1(J),C2(J),J=1,IMAX)

WRITE(6,2002)

WRITE(6,2000)(J,SS(J),CC(J),J=1,MAXI)

MAXII = MAXI + 1

INITIALIZE THE AS, AC, BS AND BC ARRAYS

DO 199 J=1,1452

AS(J) = .0D0

BS(J) = .0D0

AC(J) = .0D0

199 BC(J) = .0D0



INITIALIZE THE A1 AND A2 ARRAYS

```
DO 200 J=1,144
  A1(J) = .000
200 A2(J) = .000
  NNMAX = MAXI
  LLMAX = MAXI
  NNM = NNMAX + 1
  LLM = 2*LLMAX - 1
  AP = 0.500*ALFA
  ALFAP = 0.101/AP
  ALFA4 = 0.201/(0.201*Z + ALFA)
```

USING THE IS AND IC INTEGRALS FOUND ABOVE EVALUATE AS(NU,  
LAMDA,2) AND AC(NU,LAMDA,2)

```
DO 201 NN=1,NNMAX
  SSN = SS(NN)
  CCN = CC(NN)
  AP = AP*ALFAP
  F = 0.101
  ALFA4P = 0.101
DO 201 LL=1,LLMAX
  ALFA4P = ALFA4P*ALFA4
  F = F*DFLOAT(LL)
  IF((NN+LL.LT.4).OR.(NN+LL.GT.IMAX)) GO TO 201
  INA = NN + NNM*(LL + LLM)
  TAA = F*ALFA4P*AP
  AS(INA) = TAA*SSN
  AC(INA) = TAA*CCN
201 CONTINUE
  N1MAX = MAXII
  L1MAX = MAXII
  IMAXI = IMAX + 1
```

USING THE I1 AND I3 INTEGRALS FOUND ABOVE EVALUATE A1(NU,  
LAMDA,2) AND A2(NU,LAMDA,2)

```
DO 202 NN=1,N1MAX
DO 202 LL=1,L1MAX
  IF((NN+LL.GT.IMAXI).OR.(NN+LL.LT.5)) GO TO 202
```



```

    IN12 = NN + N1MAX*(LL - 1)
    CALL A12SUM(NN,LL,AA,S1)
    A1(IN12) = AA
    CALL A12SUM(NN,LL,AA,C2)
    A2(IN12) = AA
202 CONTINUE
    NNMAX = MAXII
    LLM1 = LLMAX - 1
    NLM = NNMAX*LLMAX - 1
    NNM = NNMAX - 1
    LNM = NNMAX*(LLMAX + 1) - 2

    USING THE RECURSION RELATIONS EVALUATE AS(NU,LAMDA,1),
    AC(NU,LAMDA,1), BS(NU,LAMDA,1) AND BC(NU,LAMDA,1)

    DO 203 NN=2,NNMAX
    DO 203 LL=1,LLMAX
    IF((NN+LL.GT.IMAXI).OR.(NN+LL.LT.5)) GO TO 203
    IN1 = NN + NNMAX*(LL + LLM1)
    INA1 = IN1 + NLM
    INLA = LL + N1MAX*(NN - 1)
    INNA = LL + 1 + N1MAX*(NN - 2)
    AS(IN1) = AS(INA1) + A1(INLA) - A1(INNA)
    AC(IN1) = AC(INA1) + A2(INLA) - A2(INNA)
    IF((NN.LT.3).OR.(LL.LT.2).OR.(NN+LL.LT.6).OR.(NN.GT.
1NNM).OR.(LL.GT.LLM)) GO TO 203
    INB1 = IN1 + LNM
    INLB = LL - 1 + N1MAX*NN
    INNB = LL + 2 + N1MAX*(NN - 3)
    BS(IN1) = ( AS(INB1) + A1(INLB) - A1(INNB))/ .3D1
    BC(IN1) = ( AC(INB1) + A2(INLB) - A2(INNB))/ .3D1
203 CONTINUE
    MMMAX = MAXI
    MAXI3 = IMAX + 3
    MMM = MMMAX - 2
    NN1 = 2*(NNMAX*LLMAX - 1)
    NN2 = 2*NNMAX*LLM1
    NN3 = NNMAX*LLM - 1

```



USING THE RECURSION RELATIONS EVALUATE AS(NU,LAMDA,MU),  
AC(NU,LAMDA,MU), BS(NU,LAMDA,MU) AND BC(NU,LAMDA,MU) FOR  
MU > 2

```

DO 204 MM=4,MMMAX
FM31 = DFLOAT(MM - 3)/DFLOAT(MM + 1)
DO 204 NN=2,NNMAX
DO 204 LL=1,LLMAX
IF((NN+LL+MM.GT.MAXI3).OR.(NN+LL.LT.4)) GO TO 204
IN = NN + NNMAX*((LL - 1) + LLMAX*(MM - 1))
INN = IN - NN1
INL = IN - NN2
INN1 = IN - NN3
AS(IN) = AS(INN) + AS(INL) - BS(INNL)*.2D1
AC(IN) = AC(INN) + AC(INL) - BC(INNL)*.2D1
IF((LL.LT.2).OR.(NN.LT.3).OR.(LL+MM.LT.6).OR.(MM.GT.
1MMM)) GO TO 204
BS(IN) = ( BS(INN) + BS(INL) - AS(INNL)*.2D1)*FM31
BC(IN) = ( BC(INN) + BC(INL) - AC(INNL)*.2D1)*FM31
204 CONTINUE
RETURN
2000 FORMAT(20X,I2,2D30.16)
2001 FORMAT(////,34X,' S1',24X,' C2',//)
2002 FORMAT(////,34X,' SS',24X,' CC',//)
3000 FORMAT('-',10X,'PH1 = ',D23.16,/, '0',10X,'FR1 = ',D23.
116,/, '0',10X,'PH2 = ',D23.16,/, '0',10X,'FR2 = ',D23.16
2,/, '0',10X,'ASCL = ',D22.16,/, '-')
END

```





SUBROUTINE ZERO(ICS,J,X0,IQ)

ZERO FINDS ALL THE ZEROES OF  $\sin(A*X + B*\ln(X) + C)$  OR  $\cos(A*X + B*\ln(X) + C)$  BETWEEN  $X=XSM$  AND  $X=SLM$

IMPLICIT REAL\*8 (A-H,O-Z)

COMMON/CONST/PH1,PH2,FR1,FR2,ASCL,PI,CA,CI,B

COMMON/INT/XSM,FF,BJ,XLM

DIMENSION XO(1)

X = XSM

GO TO (21,22,21,22),ICS

21 A = FR1

CC = PH1

GO TO 1

22 A = FR2

CC = PH2

1 ARG =  $A*X + B*\ln(X) + CC$

FIND THE SMALLEST (ALGEBRAICALLY) INTEGER MULTIPLE OF PI SUCH THAT  $A*X + B*\ln(X) + C > N*PI$

ARGP = ARG/PI

ITHTA = IDINT(ARGP) - 1

IT = IABS(ITHTA)

DETERMINE WHETHER THIS ZERO STARTS A POSITIVE OR A NEGATIVE SWING OF THE FUNCTION AND RECORD THIS FACT

IQ = MOD(IT,2)

IF(IQ.EQ.0) IQ = -1

THTA = PI\*DFLOAT(ITHTA)

IF (ICS.GT.2) THTA = THTA - 0.500\*PI

FIND THE VALUE OF X CORRESPONDING TO THIS INITIAL VALUE OF THE ARGUMENT

CALL XZERO(THTA,X,A,B,CC)

XO(1) = X

REPEAT THIS PROCESS UNTIL  $X > XLM$  OR UNTIL 500 ZEROES HAVE BEEN FOUND

DO 2 J=2,500

THTA = THTA + PI

X =  $X + PI/(A + B/X)$



```

      CALL XZERO(THTA,X,A,B,CC)
      XO(J) = X
      IF (X.GT.XLM)      GO TO 3
2  CONTINUE
      J = 500
3  CONTINUE
      RETURN
      END

```

```

      SUBROUTINE XZERO(THTA,X,A,B,CC)

```

XZERO SOLVES THE EQUATION  $\text{THETA} = A * X + B * \text{LN}(X) + C$  FOR X BY AN ITERATION PROCESS

```

      IMPLICIT REAL*8 (A-H,O-Z)

```

```

      1 X1 = X*(THTA - (CC + B*(DLOG(X) - 1)))/(X*A + B)

```

IF THE LINEAR APPROXIMATION RESULTS IN A NEGATIVE ESTIMATE FOR X THE METHOD FAILS SO REPLACE THE ESTIMATE OF X BY ONE-TENTH OF THE INITIAL VALUE OF X AND REPEAT THE APPROXIMATION FINDING A NEW ESTIMATE. REPEAT THIS PROCESS UNTIL THE ESTIMATE BECOMES POSITIVE

```

      IF(X1.LE.0.0D0) X1 = 0.1D0*X
      IF (DABS(X-X1).LT.0.1D-12) GO TO 2
      X = X1
      GO TO 1
2  X = X1
      RETURN
      END

```



SUBROUTINE CSINT(ICS,M,IQ,XO,F,P)

CSINT CARRIES OUT THE NUMERICAL INTEGRATION OF THE BOUND-FREE INTEGRALS FOR  $Z > 1$

IMPLICIT REAL\*8 (A-H,O-Z)

EXTERNAL FQN,FCN,DSIN,DCOS

COMMON/MONE/C,D,FFA

COMMON/INT/XSM,FF,B0,XLM

COMMON/GEZRO/FA,B,AMP,ICC,IQI

COMMON/RHO/N

DIMENSION STS(4),TI(3),AC(4),AD(4),AES(4),XO(M)

ICC = ICS

TS = 0.000

SINT = 0.000

AES(1) = 0.101

DO 4 LL=1,3

4 AES(LL+1) = AES(LL) + P

FN = DFLOAT(N)

SINCE THE REGION WHERE THE INTEGRAND IS SIGNIFICANTLY DIFFERENT FROM ZERO IS DIFFERENT FOR DIFFERENT N, ADJUST THE POINT WHERE THE CAREFUL NUMERICAL INTEGRATION STARTS AND ENDS TO TAKE ADVANTAGE OF THIS

XS = XSM

IF(N.GT.1) XS = FF\*(FN - 0.101)\*(FN\*\*0.600)

XL = 0.2501\*FN + B0

IF(N.LE.1) GO TO 7

DO 5 J=1,M

IF(XO(J).GE.XS) GO TO 6

5 CONTINUE

6 JJ = J - 1

IF(JJ.EQ.0) JJ = 1

IQI DETERMINES WHETHER THE FUNCTION IS STARTING A POSITIVE OR NEGATIVE SWING ON THE NEXT HALF-CYCLE

IQI = MOD(JJ,2)

IF(IQI.EQ.1) IQI = IQ

IF(IQI.EQ.0) IQI = -IQ

GO TO 8



```

7 JJ = 1
  IQI = IQ
8 D = XO(JJ)
  IF (N.EQ.-1) GO TO 99
  DO 9 LL=1,4
    IF(D.EQ.0.0D0) GO TO 100
    AD(LL) = DEXP(-AES(LL)*D)/D
  GO TO 9
100 AD(LL) = 0.0D0
  9 CONTINUE
99 DO 10 J=1,M
  JI = M + 1 - J
  IF (XO(JI).LT.XL) GO TO 11
10 CONTINUE
11 IF(JJ.GE.JI) JI = M - 1
  DO 17 K=JJ,JI

```

C AND D REPRESENT SUCCESSIVE ZEROES OF THE TRUE INTEGRAND

```

C = D
D = XO(K+1)

```

FA IS THE FREQUENCY OF THE SIN FUNCTION WITH ZEROES AT C AND D

```

FA = 0.3141592653589793D1/(D - C)
FFA = FA
DIQ = DFLOAT(IQI)

```

IF THE TRUE INTEGRAND IS POSITIVE THE APPROXIMATE FUNCTION IS REDUCED IN AMPLITUDE BY 10% AND IF NEGATIVE, INCREASED BY 10%

```

AMP = 0.1D1 + 0.1D0 *DIQ
IF(N.EQ.-1) GO TO 14
DO 12 LL=1,4
  AC(LL) = AD(LL)
12 AD(LL) = DEXP(-AES(LL)*D)/D

```

FIRST THE INTEGRAL OF THE APPROXIMATE FUNCTION IS EVALUATED

```

DO 13 LL=1,4
  AE = -AES(LL)
  AEC = AC(LL)

```





```

      AED = AD(LL)
      CALL CSSUM(D,C,FA,TERM,AE,AEC,AED)
13  STS(LL) = TERM
      TS = TS +      DIQ*AMP*(STS(1) - 0.3D1*(STS(2)
1 - STS(3)) - STS(4))
      GO TO 16
14  UL = 0.1D1

FOR N=-1 THE APPROXIMATE FUNCTION MUST ALSO BE EVALUATED
NUMERICALLY
      DO 15 LL=1,3
      BL = UL
      UL = BL + P
      CALL DQG32(BL,UL,FQN,TT)
15  TI(LL) = TT
      TS = TS -      DIQ*AMP*FA*(TI(1) - 0.2D1*TI(2) + TI(3))

NEXT EVALUATE THE INTEGRAL OF THE DIFFERENCE BETWEEN THE
TRUE INTEGRAND AND THE APPROXIMATE ONE NUMERICALLY USING A
32-POINT GAUSS-LEGENDRE QUADRATURE
16  DD = DFLOAT(1 + (1 - IQI)/2)
      CC = DD + 0.1D1

B IS THE PHASE OF THE APPROXIMATE FUNCTION, SO CHOSEN TO
MAKE THE FUNCTION BEHAVE PROPERLY
      B = FA*(DD*D - CC*C)
      CALL DQG32(C,D,FCN,FG)
      SINT = SINT + FG
17  IQI = -IQI

FINALLY THE REGION FROM 0 TO XS AND FROM XL TO 100 IS INT-
TEGRATED WITHOUT USING THE APPROXIMATE FUNCTION, UTILIZING A
512-POINT GAUSS-LEGENDRE QUADRATURE
      IF (ICS.GT.2) GO TO 18
      D = X0(JJ)
      IF(D.EQ.0.0D0) GO TO 24
      CALL DQ512(0.0D0,D,DSIN,ZI)
      GO TO 25
24  ZI = 0.0D0
25  C = X0(JI+1)
      IF(C.GE.0.6D2) GO TO 20
      CALL DQ512(C,0.6D2,DSIN,UI)

```



```

      CL = 0.6D2
      GO TO 21
20  CL = C
      UI = 0.0D0
      IF(C.GE.0.1D3) GO TO 26
21  CALL DQ512(CL,0.1D3,DSIN,UJ)
      GO TO 19
18  D = X0(JJ)
      IF(D.EQ.0.0D0) GO TO 28
      CALL DQ512(0.0D0,D,DCOS,ZI)
      GO TO 29
28  ZI = 0.0D0
29  C = X0(JI+1)
      IF(C.GE.0.6D2) GO TO 22
      CALL DQ512(C,0.6D2,DCOS,UI)
      CL = 0.6D2
      GO TO 23
22  CL = C
      UI = 0.0D0
      IF(C.GE.0.1D3) GO TO 26
23  CALL DQ512(CL,0.1D3,DCOS,UJ)
      GO TO 19
26  UJ = 0.0D0

```

THE FINAL INTEGRAL IS THE SUM OF ALL THE INDIVIDUAL INTEGRATIONS

```

19  F = SINT + TS + ZI + UI + UJ
      RETURN
      END

```



SUBROUTINE CSSUM(D,C,A,TERM,AE,AEC,AED)

CSSUM FINDS THE INTEGRAL OF  $(X**N)*(EXP(-ALPHA*X))*SIN(AX+B)$   
BETWEEN SUCCESSIVE ZEROES OF THE INTEGRAND

IMPLICIT REAL\*8 (A-H,O-Z)

COMMON/RHO/N

LIM = N + 1

DEN = -DSQRT(A\*A + AE\*AE)

PH = DATAN2(A,AE)

S = 0.0D0

F = 0.1D1

DI = 0.1D1

DR = 0.1D1/DEN

PHP = PH\*DFLOAT(N+2)

FN = 0.1D1/DFLOAT(LIM)

AC = AEC

AD = AED

DO 10 I=1,LIM

FI = DFLOAT(I)

FN = FN\*FI

DI = DI\*DEN

DR = DR\*DEN

F = F\*FI

PHP = PHP - PH

AC = AC\*C

IF((AC.EQ.0.0D0).AND.(I.EQ.1)) AC = 0.1D1

AD = AD\*D

10 S = S + DSIN(PHP)\*FI\*DR\*(AD + AC)/F

TERM = FN\*S/DI

RETURN

END



SUBROUTINE DQG32(XL,XU,FCT,Y)

DQG32 IS A 32-POINT GAUSS-LEGENDRE QUADRATURE WHICH INTEGRATES AN EXTERNALLY DEFINED FUNCTION FCT BETWEEN THE LIMITS XL AND XU

DESCRIPTION OF PARAMETERS

XL: LOWER BOUND OF THE INTERVAL

XU: UPPER BOUND OF THE INTERVAL

FCT: NAME OF THE EXTERNALLY DEFINED FUNCTION TO BE INTEGRATED

Y: RESULTING INTEGRAL VALUE

DOUBLE PRECISION XL,XU,Y,A,B,C,FCT

DEFINING A AND B ENABLES THE VARIABLE TO BE CHANGED TO CONFORM WITH THE -1,+1 INTERVAL REQUIRED OF THE GAUSS-LEGENDRE QUADRATURE

A= .5D0\*(XU+XL)

B=XU-XL

C= .49863193092474078D0\*B

Y= .35093050047350483D-2\*(FCT(A+C)+FCT(A-C))

C= .49280575577263417D0\*B

Y=Y+ .8137197355452835D-2\*(FCT(A+C)+FCT(A-C))

C= .48238112779375322D0\*B

Y=Y+ .12696032654631030D-1\*(FCT(A+C)+FCT(A-C))

C= .46745303795886984D0\*B

Y=Y+ .17136931456510717D-1\*(FCT(A+C)+FCT(A-C))

C= .44816057788302606D0\*B

Y=Y+ .21417949011113340D-1\*(FCT(A+C)+FCT(A-C))

C= .42468380686628499D0\*B

Y=Y+ .25499029531188088D-1\*(FCT(A+C)+FCT(A-C))

C= .39724189798397120D0\*B

Y=Y+ .29342046739267774D-1\*(FCT(A+C)+FCT(A-C))

C= .36609105937014484D0\*B

Y=Y+ .32911111388180923D-1\*(FCT(A+C)+FCT(A-C))

C= .33152213346510760D0\*B

Y=Y+ .36172897054424253D-1\*(FCT(A+C)+FCT(A-C))

C= .29385787862038116D0\*B

Y=Y+ .39096947893535153D-1\*(FCT(A+C)+FCT(A-C))

C= .25344995446611470D0\*B

Y=Y+ .41655962113473378D-1\*(FCT(A+C)+FCT(A-C))

C= .21067563806531767D0\*B





```

Y=Y+.43826046502201906D-1*(FCT(A+C)+FCT(A-C))
C=.16593430114106382D0*B
Y=Y+.45586939347881942D-1*(FCT(A+C)+FCT(A-C))
C=.11964368112606854D0*B
Y=Y+.46922199540402283D-1*(FCT(A+C)+FCT(A-C))
C=.7223598079139825D-1*B
Y=Y+.47819360039637430D-1*(FCT(A+C)+FCT(A-C))
C=.24153832843869158D-1*B
Y=B*(Y+.48270044257363900D-1*(FCT(A+C)+FCT(A-C)))
RETURN
END

```

DOUBLE PRECISION FUNCTION FQN(Z)

```

FQN EVALUATES THE APPROXIMATE FUNCTION AT GIVEN Z FOR RHO=-1
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/MONE/C,D,FA
FQN = (DEXP(-C*Z) + DEXP(-D*Z))/(Z*Z + FA*FA)
RETURN
END

```

DOUBLE PRECISION FUNCTION FCN(Z)

```

FCN EVALUATES THE DIFFERENCE BETWEEN THE TRUE INTEGRAND AND
THE APPROXIMATE ONE FOR GIVEN Z
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/CONST/PH1,PH2,FR1,FR2,ASCL,PI,CA,CI,AA
COMMON/GEZRO/FA,B,F,ICS,IQI
COMMON/RHO/N
GO TO (1,2,1,2),ICS
1 FR = FR1
  PH = PH1
  P = ASCL
  GO TO 3
2 FR = FR2

```



```

PH = PH2
P = 0.1D1
3 ARGF = FR*Z + AA*DLOG(Z) + PH
  ARGH = FA*Z + B
  S = 0.1D1 - DEXP(-P*Z)
  ZN = 0.1D1/(Z*Z)
  NN = N + 2
  DO 6 I=1,NN
6  ZN = ZN*Z
  ENV = S*S*S*DEXP(-Z)*ZN
  IF (ICS.GT.2) GO TO 4
  FCN = ENV*(DSIN(ARGF) - F*DSIN(ARGH))
  GO TO 5
4  FCN = ENV*(DCOS(ARGF) - F*DSIN(ARGH))
5  RETURN
  END

```



SUBROUTINE DQ512(C,D,FCT,Y)

DQ512 IS A 512-POINT GAUSS-LEGENDRE QUADRATURE WHICH EVALUATES THE BOUND-FREE INTEGRALS BETWEEN THE LIMITS C AND D. THE EXTERNALLY DEFINED FUNCTION FCT IS EITHER SIN OR COS. LOCATION OF THE SAMPLE POINTS AND THE CORRESPONDING WEIGHT FACTORS ARE READ INTO THE MAIN PROGRAM FROM AN EXTERNAL SOURCE.

IMPLICIT REAL\*8 (A-H,O-Z)

COMMON/L512/X(256),A(256)

COMMON/CONST/PH1,PH2,FR1,FR2,ASCL,PI,CA,CT,AA

COMMON/GEZRO/FA,B,AMP,ICS,IQI

COMMON/RHO/N

GO TO (1,2,1,2),ICS

1 FR = FR1

PH = PH1

P = ASCL

GO TO 3

2 FR = FR2

PH = PH2

P = 0.1D1

3 Y = 0.0D0

CHANGE THE VARIABLE SO THAT THE INTEGRATION LIMITS BECOME (-1,+1)

DPC = 0.5D0\*(D + C)

DMC = 0.5D0\*(D - C)

DO 4 I=1,256

XDC = X(I)\*DMC

ZP = DPC + XDC

ZM = DPC - XDC

ZMN = 0.1D1/(ZM\*ZM)

ZPN = 0.1D1/(ZP\*ZP)

NN = N + 2

DO 5 J=1,NN

ZMN = ZMN\*ZM

5 ZPN = ZPN\*ZP

SP = 0.1D1 - DEXP(-P\*ZP)

SM = 0.1D1 - DEXP(-P\*ZM)



```

ENVP = SP*SP*SP*DEXP(-ZP)*ZPN
ENVM = SM*SM*SM*DEXP(-ZM)*ZMN
ARGP = FR*ZP + AA*DLOG(ZP) + PH
ARGM = FR*ZM + AA*DLOG(ZM) + PH
4 Y = Y + A(I)*(ENVP*FCT(ARGP) + ENVM*FCT(ARGM))
Y = Y*DMC
RETURN
END

```





```
SUBROUTINE HINT(S1,C2,SS,CC,IMAX,MAXI)
```

```
HINT EVALUATES THE BOUND-FREE INTEGRALS FOR THE CASE Z=1
```

```
IMPLICIT REAL*8 (A-H,O-Z)
```

```
EXTERNAL FACT
```

```
COMMON/CONST/PH1,PH2,FR1,FR2,ASCL,PI,CA,CI,AAA
```

```
1 DIMENSION RHO1(4),RHO2(4),THTAS1(4),THTAC1(4),  
THTAS2(4),THTSC2(4)
```

```
DIMENSION S1(IMAX),C2(IMAX),SS(MAXI),CC(MAXI)
```

```
F1 = FR1**2
```

```
F2 = FR2**2
```

```
DO 1 K=1,4
```

```
A = DFLOAT(K - 1)
```

```
RHO1(K) = DSQRT((0.1D1 + A*ASCL)**2 + F1)
```

```
RHO2(K) = DSQRT((0.1D1 + A)**2 + F2)
```

```
THTAS1(K) = DARSIN(FR1/RHO1(K))
```

```
THTAC1(K) = DARCCOS((0.1D1 + A*ASCL)/RHO1(K))
```

```
THTAS2(K) = DARSIN(FR2/RHO2(K))
```

```
1 THTAC2(K) = DARCCOS((0.1D1 + A)/RHO2(K))
```

```
1 S1(1) = DATAN(FR1) - 0.3D1*(DATAN(FR1/(0.1D1 + ASCL))  
2 - DATAN(FR1/(0.1D1 + 0.2D1*ASCL)))  
2 - DATAN(FR1/(0.1D1 + 0.3D1*ASCL))
```

```
1 C2(1) = 0.15D1*DLOG(((0.1D1 + ASCL)**2 + F1)/((0.1D1  
2 + 0.2D1*ASCL)**2 + F1)) + 0.5D0*DLOG(((0.1D1  
2 + 0.3D1*ASCL)**2 + F1)/(0.1D1 + F1))
```

```
1 SS(1) = DATAN(FR2) - 0.3D1*(DATAN(FR2/0.2D1)  
1 - DATAN(FR2/0.3D1)) - DATAN(FR2/0.4D1)
```

```
1 CC(1) = 0.15D1*DLOG((0.4D1 + F2)/(0.9D1 + F2)) +  
1 0.5D0*DLOG((0.16D2 + F2)/(0.1D1 + F2))
```

```
DO 2 J=2,IMAX
```

```
I = J - 1
```

```
FI = DFLOAT(I)
```

```
FCT = FACT(J - 2)
```

```
1 S1(J) = FCT*(DSIN(FI*THTAS1(1))/RHO1(1)**I  
2 - 0.3D1*(DSIN(FI*THTAS1(2))/RHO1(2)**I  
3 - DSIN(FI*THTAS1(3))/RHO1(3)**I)  
3 - DSIN(FI*THTAS1(4))/RHO1(4)**I)
```

```
1 C2(J) = FCT*(DCOS(FI*THTAC1(1))/RHO1(1)**I  
2 - 0.3D1*(DCOS(FI*THTAC1(2))/RHO1(2)**I  
3 - DCOS(FI*THTAC1(3))/RHO1(3)**I)  
3 - DCOS(FI*THTAC1(4))/RHO1(4)**I)
```

```
IF(J.GT.MAXI) GO TO 2
```



```

      SS(J) = FCT*(DSIN(FI*THTAS2(1))/RHO2(1))*I
1      - 0.3D1*(DSIN(FI*THTAS2(2))/RHO2(2))*I
2      - DSIN(FI*THTAS2(3))/RHO2(3))*I)
3      - DSIN(FI*THTAS2(4))/RHO2(4))*I)

      CC(J) = FCT*(DCOS(FI*THTAC2(1))/RHO2(1))*I
1      - 0.3D1*(DCOS(FI*THTAC2(2))/RHO2(2))*I
2      - DCOS(FI*THTAC2(3))/RHO2(3))*I)
3      - DCOS(FI*THTAC2(4))/RHO2(4))*I)

2 CONTINUE

      RETURN

      END

```



SUBROUTINE A12SUM(NU,LMDA,AA,VAL)

A12SUM EVALUATES A1(NU,LAMDA,2) OR A2(NU,LAMDA,2) USING I1  
OR I3, RESPECTIVELY

IMPLICIT REAL\*8 (A-H,O-Z)

DIMENSION VAL(1)

COMMON/TRM/ALFA,ETA

COMMON/ATNO/Z

ALFA2 = Z + ALFA

FCTR = 0.2D1\*ALFA2/(0.2D1\*Z + ALFA)

NU1 = NU + 1

NL = NU + LMDA

F = 0.1D1/DFLOAT(NU)

FCT = 0.1D1/FCTR

TVAL = 0.0D0

DO 10 I=1,NU

F = F\*DFLOAT(NU1 - I)

FCT = FCT\*FCTR

10 TVAL = TVAL + FCT\*VAL(NL-I)\*F

AA = TVAL/ALFA2\*\* (NL-2)

RETURN

END



SUBROUTINE PHASE(AS,AC,BS,BC,MAXI,HS,HC,E)

PHASE COMPILES THE MATRIX ELEMENTS  $\langle S|(H-E)|CHI(I)\rangle$  AND  
 $\langle C|(H-E)|CHI(I)\rangle$

IMPLICIT REAL\*8 (A-H,O-Z)

COMMON/TRM/ALFA,ETA

COMMON/ATNO/Z

COMMON/INDEX/NI,NJ,LI,LJ,MI,MJ,IS

DIMENSION AS(1),AC(1),BS(1),BC(1)

DIMENSION NU(26),LMDA(26),MU(26),COEF(26)

FN = DFLOAT(NJ)

FL = DFLOAT(LJ)

FM = DFLOAT(MJ)

SET THE VALUES OF NJ, LAMDA, MU AND THE COEFFICIENTS FOR  
EACH OF THE 26 TERMS OF THE MATRIX ELEMENT

NU( 1) = LJ + 1

NU( 3) = NU(1)

NU( 4) = NU(1)

NU( 6) = NU(1)

NU( 8) = NU(1)

NU( 9) = NU(1)

NU(19) = NU(1)

LMDA(12) = NU(1)

LMDA(26) = NU(1)

NU( 2) = LJ

LMDA(17) = NU(2)

NU(21) = NU(2)

NU( 5) = LJ + 2

NU(20) = NU(5)

NU(22) = NU(5)

LMDA(10) = NU(5)

LMDA(11) = NU(5)

LMDA(14) = NU(5)

LMDA(15) = NU(5)

LMDA(16) = NU(5)

LMDA(18) = NU(5)





```

LMDA(24) = NU(5)
NU( 7) = LJ - 1
NU(10) = NJ + 1
NU(12) = NU(10)
NU(13) = NU(10)
NU(15) = NU(10)
NU(17) = NU(10)
NU(18) = NU(10)
NU(23) = NU(10)
LMDA( 3) = NU(10)
LMDA(22) = NU(10)
NU(11) = NJ
NU(25) = NU(11)
LMDA( 8) = NU(11)
NU(14) = NJ + 2
NU(24) = NU(14)
NU(26) = NU(14)
LMDA( 1) = NU(14)
LMDA( 2) = NU(14)
LMDA( 5) = NU(14)
LMDA( 6) = NU(14)
LMDA( 7) = NU(14)
LMDA( 9) = NU(14)
LMDA(20) = NU(14)
NU(16) = NJ - 1
LMDA( 4) = NJ + 3
LMDA(19) = LMDA(4)
LMDA(21) = LMDA(4)
LMDA(13) = LJ + 3
LMDA(23) = LMDA(13)
LMDA(25) = LMDA(13)
MU( 1) = MJ + 2
MU( 2) = MU(1)
MU( 3) = MU(1)
MU( 7) = MU(1)
MU( 8) = MU(1)

```



```

MU(10) = MU(1)
MU(11) = MU(1)
MU(12) = MU(1)
MU(16) = MU(1)
MU(17) = MU(1)
MU( 4) = MJ
MU( 5) = MU(4)
MU( 6) = MU(4)
MU(13) = MU(4)
MU(14) = MU(4)
MU(15) = MU(4)
MU(19) = MU(4)
MU(20) = MU(4)
MU(21) = MU(4)
MU(22) = MU(4)
MU(23) = MU(4)
MU(24) = MU(4)
MU(25) = MU(4)
MU(26) = MU(4)
MU( 9) = MJ + 1
MU(18) = MU(9)
COEF( 1) = -0.25D0*ALFA**2 - E
COEF(10) = COEF( 1)
COEF( 2) = 0.5D0*ALFA*(FL + 0.1D1) - Z
COEF(12) = COEF( 2)
COEF( 3) = 0.5D0*ALFA*(FN + 0.1D1) - Z
COEF(11) = COEF( 3)
COEF( 4) = 0.5D0*ALFA*FM
COEF( 5) = COEF(4)
COEF(13) = COEF( 4)
COEF(14) = COEF(4)
COEF(19) = -COEF( 4)
COEF(20) = -COEF( 4)
COEF(23) = -COEF(4)
COEF(24) = -COEF(4)
COEF( 6) = -FM*(FM + FN + FL + 0.1D1)

```



```

COEF(15) = COEF( 6)
COEF( 7) = -0.5D0*FL*(FL + 0.1D1)
COEF(17) = COEF( 7)
COEF( 8) = -0.5D0*FN*(FN + 0.1D1)
COEF(16) = COEF( 8)
COEF( 9) = 0.1D1
COEF(18) = COEF( 9)
COEF(21) = FM*FL
COEF(26) = COEF(21)
COEF(22) = FM*FN
COEF(25) = COEF(22)
IF(15.EQ.0) GO TO 10

```

CHANGE THE SIGNS OF THE LAST 13 TERMS FOR THE TRIPLET CASE

```

DO 1 I=10,18
1 COEF(I) = -COEF(I)
DO 2 I=23,26
2 COEF(I) = -COEF(I)
10 LLMAX = MAXI
NNMAX = MAXI + 1
HS = 0.0D0
HC = 0.0D0
DO 20 K=1,18
IN = NU(K) + 2 + NNMAX*(LMDA(K) + LLMAX*MU(K) - 1)
HS = HS + AS(IN)*COEF(K)
HC = HC + AC(IN)*COEF(K)
20 CONTINUE
DO 30 K=19,26
IN = NU(K) + 2 + NNMAX*(LMDA(K) + LLMAX*MU(K) - 1)
HS = HS + BS(IN)*COEF(K)
HC = HC + BC(IN)*COEF(K)
30 CONTINUE
RETURN
END

```



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ORIGINATING ACTIVITY (Corporate author)

Naval Postgraduate School  
Monterey, California 93940

2a. REPORT SECURITY CLASSIFICATION

Unclassified

2b. GROUP

REPORT TITLE

Application of the Harris Expansion Method to the Elastic S-wave Scattering  
of Electrons by Hydrogen Atoms and by Singly Ionized Helium

DESCRIPTIVE NOTES (Type of report and, inclusive dates)

Doctor of Philosophy Thesis: December 1972

AUTHOR(S) (First name, middle initial, last name)

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REPORT DATE

December 1972

7a. TOTAL NO. OF PAGES

173

7b. NO. OF REFS

58

CONTRACT OR GRANT NO.

9a. ORIGINATOR'S REPORT NUMBER(S)

PROJECT NO

9b. OTHER REPORT NO(S) (Any other numbers that may be assigned  
this report)

DISTRIBUTION STATEMENT

Approved for public release; distribution unlimited.

SUPPLEMENTARY NOTES

12. SPONSORING MILITARY ACTIVITY

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ABSTRACT

The Harris expansion method is applied to the elastic s-wave scattering of low energy electrons from hydrogen atoms and singly ionized helium atoms. The trial wave functions are Hylleraas functions of 22, 34, 50 and 70 parameters. It is found that reasonably accurate values of e-H phase shifts can be calculated but that e-He<sup>+</sup> phase shifts are substantially less reliable. It is shown that the Harris method gives an accurate depiction of the location, but not the width, of the scattering resonances. Singlet and triplet s-wave phase shifts for e-H and e-He<sup>+</sup> scattering are compared with the results of other calculations and H<sup>-</sup> and He S state energy levels including the auto-ionizing levels are presented and compared with other calculations and with experiment. It is tentatively concluded that the Harris method does not work on systems whose long range potential is of the Coulomb type.





14 KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Scattering Theory						
Atomic Scattering						
Electron-Hydrogen Scattering						
Electron-Helium Ion Scattering						
Harris Expansion Method						
Resonances						
Scattering Resonances						
Auto-ionization States						



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